Operator-Theoretic Framework for Forecasting Nonlinear Time Series with Kernel Analog Techniques

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Abstract

Kernel analog forecasting (KAF), alternatively known as kernel principal component regression, is a kernel method used for nonparametric statistical forecasting of dynamically generated time series data. This paper synthesizes descriptions of kernel methods and Koopman operator theory in order to provide a single consistent account of KAF. The framework presented here illuminates the property of the KAF method that, under measure-preserving and ergodic dynamics, it consistently approximates the conditional expectation of observables that are acted upon by the Koopman operator of the dynamical system and are conditioned on the observed data at forecast initialization. More precisely, KAF yields optimal predictions, in the sense of minimal root mean square error with respect to the invariant measure, in the asymptotic limit of large data. The presented framework facilitates, moreover, the analysis of generalization error and quantification of uncertainty. Extensions of KAF to the construction of conditional variance and conditional probability functions are also shown. Illustrations of various aspects of KAF are provided with applications to simple examples, namely a periodic flow on the circle and the chaotic Lorenz 63 system.

Keywords:
Statistical forecasting, kernel methods, conditional expectation, Koopman operators

1. Introduction

Forecasting dynamically generated time series is a challenging problem that often requires statistical methods, especially when the underlying equations are either unknown or computationally intractable. Data-driven such methods have been sought after at least since Lorenz attempted to use naturally occurring historical analogs for climate predictions in the 1960’s [1]. That early attempt was limited in success, but larger data sets and improved computing resources have made more recent analog-based nonparametric methods more viable [2–6]. Various types of ensemble analog forecasting are employed in short-term meteorological forecasts [7, 8], and versions of analog forecasting that utilize kernels have been shown to have predictive value for certain weather and climate phenomena [9–11].

While naturally occurring analogs may be a point of emphasis for nonparametric methods in physical science applications, abstract statistical structures are the focus when situated in a more general machine learning context. Common nonparametric machine learning techniques include multilayer perceptrons [12], Bayesian neural networks [13], classification and regression trees (CART), and a variety of kernel methods [14]. Although each of these methods can provide value in unique ways to specific problems, kernel methods are particularly well suited to problems where there may be a natural, a priori, notion of similarity between data points. Since analog methods rely on the possibility that the relevance of any historical analog to present day conditions can be quantitatively determined, formal understanding of such methods can improve when they are cast within the larger framework of kernel methods.

Kernel methods constitute a class of algorithms that perform classical calculations in a rich functional feature space in order to extract and predict nonlinear patterns. This central idea, commonly referred to as “the kernel trick”, was first proposed in 1964 [15], was popularized with the invention of nonlinear support vector machines (SVMs) in 1992 [16], and has since spread to a variety of machine learning applica-
tions [17]. Kernel methods for regression, such as support vector regression (SVR) [18], kernel ridge regression (KRR) [19], and kernel principal components regression (KPCR) [20], may be applied to appropriately lagged signals to produce time series forecasts, such as with SVR forecasting [21], KRR forecasting [22], and KPCR forecasting [20]. Such kernel forecasting methods have been frequently used in finance and econometrics [23], and have recently found use in climate science [6, 9–11], where they were termed kernel analog forecasting (KAF).

Statistical learning theory [24] is the standard theoretical framework for deriving and analyzing kernel methods, among other machine learning algorithms. The learning guarantees and estimates of rates of convergence are well known when the underlying data are independently and identically distributed [25]. For time series, where the i.i.d. assumption is generally not valid, an extension of the standard i.i.d. statistical learning framework to that of stochastic processes has yielded softer guarantees that depend on mild conditions on the stationarity of the system [26, 27]. Although trajectories of a dynamical system can be viewed as a special case of a stochastic process [28], it is also worthwhile to employ the typical measure and operator-theoretic perspectives of modern dynamical systems theory [29], where the induced action of the dynamical system on an intrinsically linear space of observables is given a more prominent role. This operator-theoretic perspective, although widespread in the study of dynamical systems [30], has yet to be fully exploited in conjunction with kernel forecasting methods.

The main contribution of this paper is a rigorous reformulation of KAF techniques within the framework of operator-theoretic ergodic theory and statistical learning theory. This view relies on the equivalence of forecasts with conditional expectation or, alternatively, geometric projection, both of which draw on the rich theory of functional analysis. One benefit from such a perspective is that it turns the problem of error analysis into the well studied problem of convergence in Hilbert spaces. Another benefit to this approach is that it demystifies the “kernel trick” somewhat. In particular, from the perspective put forward in this paper, the kernel trick is nothing more than the calculation of the adjoint of the canonical inclusion map between two well-chosen Hilbert spaces. A third benefit is the modularity and extensibility that comes from casting kernel forecasting algorithms as a composition of operators applied to a careful choice of observable. In particular, by expressing forecasts as a composition of a regressor operator and the Koopman operator [31], the latter being a construct representing the action of evolving forward in time, features of the statistics and the dynamics are more easily separated and studied independently. For example, approximations of Koopman and the related transfer operators has been the subject of recent research [32–36], and may be combined with approximations of the regressor operator to yield new formulations. Moreover, with appropriate choices of the response observable, forecasts can be obtained not just for the conditional mean of an observed quantity, but also that quantity’s conditional variance and higher order moments, which are important for uncertainty quantification. Conditional probability may also be approximated and predicted with a kernel analog approach. In this analysis, reproducing kernel Hilbert spaces (RKHSs) [37] play a central role as ambient hypothesis spaces of functions, with enough structure to enable an explicit representation of the forecasting function (also known as target function) in a fully empirical manner.

This paper is organized as follows. Section 2 introduces the forecasting problem under study, and describes the KAF framework. Section 3 studies the generalization error of constructed forecasts, paying particular attention on how to quantify the discrepancy between empirical and ideal forecasts. Our main result on the convergence of KAF to the conditional expectation is stated as Theorem 3 in that section. Section 4 introduces a few extensions, including KRR, conditional variance, and conditional probability. In Section 5 we provide general guidelines for choosing the kernel. Section 6 shows the result of applying KAF to two examples, namely a periodic flow on the circle and the chaotic Lorenz 63 (L63) system [38]. Section 7 provides our principal conclusory remarks, and examines the applicability of KAF to various real-world problems.

2. Kernel analog forecasting (KAF) techniques

In this section, we describe the mathematical framework underlying the KAF approach introduced in [6]. We start from a general formulation of forecasting as error minimization (Section 2.1), and gradually build onto that various dynamical systems and functional analytic tools, leading (in Section 2.4) to the construction of the RKHS-based KAF target function. It should be noted that our exposition differs substantially from [6], which focuses heavily on RKHS interpolation theory from the outset. In particular, an advantage of the perspective put forward here is that the RKHS formalism emerges as a natural consequence of seeking target functions in an explicitly constructible ambient hypothesis space with
2.1. Mathematical background

Measure-theoretic framework. In the measure-theoretic setup that we wish to pursue here, the primary object is a probability space \( (\Omega, \mathcal{F}, \rho) \), where \( \Omega \) is the space of all possible initial states, \( \mathcal{F} \) is a \( \sigma \)-algebra of distinguished subsets of \( \Omega \), and \( \rho : \mathcal{F} \to \mathbb{R} \) is a probability measure. We also have a measurable covariate space \( (X, \Sigma) \), a measurable response space \( (Y, \mathcal{Y}) \), and, for each function \( f \), a data-producing measurable function \( X_f : \Omega \to X \) and \( Y_f : \Omega \to Y \). By data-producing, we mean the covariate and response data, \( x_t \) and \( y_t \), are regarded as the output of \( X_f \) and \( Y_f \), respectively, so that \( x_t = X_f(\omega) \) and \( y_t = Y_f(\omega) \) for some \( \omega \in \Omega \). The space \( Y \) is assumed to be a Hilbert space over the complex numbers, whose inner product \( \langle \cdot, \cdot \rangle \) is a common such functional; given this assumption, the mean square error is a common such functional, \( \langle \cdot, \cdot \rangle \), is taken to be conjugate-linear in its first argument. Note that we do not require that the space \( X \) be linear.

The task of forecasting is to produce a measurable function \( f : X \to Y \) for any given lead time \( \tau \geq 0 \), referred to as the target function, such that \( f \circ X_f \) approximates \( Y_{1+\tau} \). A heuristic for selecting such an approximation is the variational approach, wherein \( f \) is viewed as a minimizer of some global measure of error. The mean square error is a common such functional, given, as we will see below, its connection to Hilbert space theory. In particular, we regard \( Y_f \) as an element of the space \( L^2(\rho) \) of functions \( \Omega \to Y \) that are square-integrable with respect to \( \rho \). The target function \( f \), meanwhile, is sought in the space \( L^2(\rho_X) \) of functions \( f : X \to Y \) that are square-integrable with respect to \( \rho_X \), where \( \rho_X \) is the pushforward of \( \rho \) along \( X_f, \rho_X(S) = \rho(X_f^{-1}(S)) \) for all \( S \in \Sigma \). This implies that \( f \circ X_f = \rho_X \)-measurable functions in \( L^2(\rho_X) \).

In what follows, \( L^2(\rho) \) will denote the Hilbert space of equivalence classes of functions in \( \mathbb{L}^2(\rho) \) taking \( \rho \)-a.e. equal values, equipped with the standard inner product \( \langle g_1, g_2 \rangle_{L^2(\rho)} = \int \langle g_1(\omega), g_2(\omega) \rangle_Y \, d\rho(\omega) \). We define the \( L^2(\rho_X) \) Hilbert spaces associated with \( \mathbb{L}^2(\rho_X) \) analogously. As is customary, we will oftentimes identify functions in \( L^2 \) with their corresponding \( L^2 \) equivalence classes, but for the purpose of constructing concrete target functions we will keep elements of these spaces distinct. The mean square error of the target function \( f \), given a lead time \( \tau \geq 0 \), may then be defined as

\[
\| f \circ X - Y_{1+\tau} \|_{L^2(\rho)}^2 = \int_{\Omega} \| f \circ X(\omega) - Y_{1+\tau}(\omega) \|_Y^2 \, d\rho(\omega).
\]

Dynamical system framework. A dynamical system on the space \( \Omega \) is represented by a semigroup of measurable maps, \( A_t : \Omega \to \Omega \tau \), which evolve an initial state \( \omega_0 \) to a new state \( \omega_t \). The function \( X_t \) may then be represented by \( X \circ A_t \), where \( X : \Omega \to X \). The response function \( Y_{1+\tau} \) can be similarly broken up, but with the added step of using the flow map semigroup properties to split up \( A_t \) into \( A_t \circ A_s \) resulting in the expression \( Y_{1+\tau} = (Y \circ A_t) \circ A_s \), where \( Y : \Omega \to Y \). It is frequently useful to express the composition \( Y \circ A_t \) as the act of applying an operator \( U_t \), known as the Koopman operator [39], on measurable \( Y \)-valued functions on \( \Omega \), so that \( U_t Y = Y \circ A_t \). Note that, unlike \( A_t \), \( U_t \) is an intrinsically linear operator.

Henceforth, we will assume that the dynamical system is measure-preserving; that is, the pushforward measure of \( \rho \) along \( A_t \), denoted by \( \rho_t \), is constant with respect to time, so that we may write \( \rho_t = \rho \) for all times \( t \geq 0 \). With such an assumption, the Koopman operator on measurable functions extends to a unitary operator on \( L^2(\rho) \), which we will denote using the same symbol \( U_t \). Moreover, the mean square error is independent of the initialization time \( t \), and is expressed as

\[
\| f \circ X - U_t Y \|_{L^2(\rho)}^2.
\]

Conditional expectation. The random variable \( X \) induces a sub-\( \sigma \)-algebra \( \mathcal{G} \subset \mathcal{F} \), defined by \( \mathcal{G} = X^{-1}(\Sigma_X) \). This means that every function \( g : \Omega \to Y \) that is measurable with respect to \( \mathcal{G} \) is such that \( g = f \circ X \) for some \( f : X \to Y \). Thus, \( \mathcal{G} \)-measurable functions can be thought of as being “coarser” than \( \mathcal{F} \)-measurable functions, in the sense that they necessarily take constant values on subsets of \( \Omega \) where \( X \) is constant. We will denote the Hilbert subspace of \( L^2(\rho) \) consisting of \( \mathcal{G} \)-measurable equivalence classes of functions by \( L^2(\rho, \mathcal{G}) \).

It is a consequence of the Radon-Nikodym theorem that for \( U_t Y \in L^2(\rho) \), there exists a unique \( \mathcal{G} \)-measurable element \( Z_t \circ X \in L^2(\rho) \), such that for all \( g \in L^2(\rho, \mathcal{G}) \),

\[
\langle g, U_t Y \rangle_{L^2(\rho)} = \langle g, Z_t \circ X \rangle_{L^2(\rho)}.
\]

It follows from this property that \( Z_t \circ X \) is the unique element in \( L^2(\rho) \), or, equivalently, that \( Z_t \) the unique element in \( L^2(\rho_X) \), that minimizes the mean square error...
in (1). We shall refer to the composition $Z_{\tau} \circ X$ as the conditional expectation $\mathbb{E}[U \mid X]$ and to $Z_{\tau}$ as the regression function. It follows from the Hilbert space projection theorem that $\mathbb{E}[U \mid X]$ has the geometrical interpretation of being the orthogonal projection of $U$ onto $L^2(\rho \circ \varphi_\tau)$. That is,

$$\mathbb{E}[U \mid X] = P_{L^2(\rho \circ \varphi_\tau)} U,$$

where $P_{L^2(\rho \circ \varphi_\tau)} : L^2(\rho) \rightarrow L^2(\rho \circ \varphi_\tau)$ is the orthogonal projection mapping into $L^2(\rho \circ \varphi_\tau)$.

By virtue of its error-minimizing properties, it is natural to seek forecasting algorithms producing target samples of $X$ and $Y$ along a dynamical trajectory, without requiring prior knowledge of the underlying equations of motion.

### 2.2. Hypothesis spaces

#### Learning framework.

Constructing the target function requires distinguishing between the spaces $L^2(\rho)$ and $L^2(\rho \circ \varphi_\tau)$, which we do by way of the linear map $\iota : \mathbb{L}^2(\rho_X) \rightarrow L^2(\rho_X)$ that associates each concrete function $f$ to its equivalence class $\iota f$. The mean square error is then represented with the functional $E_{\iota} : \mathbb{L}^2(\rho_X) \rightarrow \mathbb{R}$, known as the generalization error in machine learning contexts [25], defined by

$$E_{\iota}(f) := \| f \circ X - U \|_{\mathbb{L}^2(\rho_X)}^2.$$  

The Hilbert space structure of $L^2(\rho)$, as well as the error-minimizing property of the conditional expectation $Z_{\tau} \circ X$, allows the generalization error to be decomposed as

$$E_{\iota}(f) = A_{\iota}(f) + \sigma_\tau,$$

where $A_{\iota}(f)$ is the excess generalization error,

$$A_{\iota}(f) := \| f - Z_{\tau} \|_{\mathbb{L}^2(\rho_X)}^2,$$

and $\sigma_\tau$ is the error intrinsic to the system and choice of covariate and response functions,

$$\sigma_\tau := \| Z_{\tau} \circ X - U \|_{\mathbb{L}^2(\rho)}^2.$$  

Since $\sigma_\tau$ does not depend on $f$, minimizing $E_{\iota}$ is equivalent to minimizing $A_{\iota}$.

#### Hypothesis space. 

Constraints on the search for a minimizer of $A_{\iota}$ are characterized in terms of a hypothesis space $\mathcal{H} \subseteq \mathbb{L}^2(\rho_X)$ of functions. When the image $H := \iota H$ is a closed and convex subset of the Hilbert space $L^2(\rho_X)$, then there exists a unique $g \in H$ such that $\inf_{g \in H} \| h - Z_{\tau} \|_{\mathbb{L}^2(\rho_X)} = \| g - Z_{\tau} \|_{\mathbb{L}^2(\rho_X)}$. Consequently, there exists $f \in H$ for which $\iota f = g$, and thus $\inf_{f \in H} \| f - Z_{\tau} \|_{\mathbb{L}^2(\rho_X)} = \| g - Z_{\tau} \|_{\mathbb{L}^2(\rho_X)}$. A sufficient condition for uniqueness of $f$ is that $\iota : \mathcal{H} \rightarrow L^2(\rho_X)$ be an injection.

#### The pseudoinverse. 

Assuming that $H$ is closed and convex in $L^2(\rho_X)$, so that there exists a well-defined orthogonal projection map $P_H : L^2(\rho_X) \rightarrow L^2(\rho_X)$ mapping into $H$, the excess generalization error may be decomposed as

$$A_{\iota}(f) = \| f - P_H Z_{\tau} \|_{\mathbb{L}^2(\rho_X)}^2 + \| (I - P_H) Z_{\tau} \|_{\mathbb{L}^2(\rho_X)}^2.$$  

The minimizer of $A_{\iota}$ over the hypothesis space $\mathcal{H}$, therefore, is found by minimizing the norm of $f - P_H Z_{\tau}$. When $\iota$ is injective on $\mathcal{H}$, then the restriction $\iota|_{\mathcal{H}}$ of $\iota$ onto $\mathcal{H}$ is invertible as a map $\iota|_{\mathcal{H}} : \mathcal{H} \rightarrow \mathcal{H}$. In such a case, the unique minimizer of $A_{\iota}$ in $\mathcal{H}$ is expressible as

$$f_{\iota|_{\mathcal{H}}} = (\iota|_{\mathcal{H}})^{-1} P_H Z_{\tau},$$

and satisfies

$$A_{\iota}(f_{\iota|_{\mathcal{H}}}) = \| (I - P_H) Z_{\tau} \|_{\mathbb{L}^2(\rho_X)}^2.$$  

We shall refer to the map $T : L^2(\rho_X) \rightarrow \mathcal{H}$, with $T = (\iota|_{\mathcal{H}})^{-1} P_H$, as the pseudoinverse of $\iota$ on $\mathcal{H}$, in analogy with the Moore-Penrose pseudoinverse of bounded, closed-range linear maps between Hilbert spaces [40]. In particular, note that $Tf = f$ for every $f \in \mathcal{H}$ and $Tg = 0$ for every $g \in H^\perp$, which shows that $T$ reduces to the Moore-Penrose pseudoinverse if $\mathcal{H}$ is a Hilbert space. In that case, the excess generalization error of the target function $f_{\iota|_{\mathcal{H}}}$ in (7) is due to the component $(I - P_H) Z_{\tau}$ of $Z_{\tau}$ in the orthogonal complement of $H$ in $L^2(\rho_X)$.

#### Ambient Hilbert space.

Explicit representations of $T$ depend on the choice of $\mathcal{H}$, and among the many such possible choices, in KAF we focus on the case where $\mathcal{H}$ is a finite-dimensional subspace of an ambient Hilbert space $\mathcal{B}$ that $\iota$ compactly embeds into $L^2(\rho_X)$. As $\iota$ is a compact operator between Hilbert spaces, its adjoint $\iota^* : L^2(\rho_X) \rightarrow \mathcal{B}$ is well-defined and compact. Consequently, the self-adjoint operator $G := \iota^* : L^2(\rho_X) \rightarrow L^2(\rho_X)$ is also compact. The spectral theorem for compact, self-adjoint operators thus guarantees the existence of an orthonormal basis $\{ \phi_i \}_{i=1}^{\infty}$ of $L^2(\rho)$ consisting...
of eigenfunctions of \( u^* \), with non-negative corresponding eigenvalues \( \lambda_i \).

By convention, we order the eigenvalues \( \lambda_i \) in decreasing order, so that the sequence \( \lambda_1, \lambda_2, \ldots \) only accumulates at zero by compactness of \( G \). Defining

\[
\psi_i = \ell^i \phi_i / \lambda_i^{1/2}
\]

for each \( \lambda_i > 0 \), and choosing \( \ell \in \mathbb{N} \) such that \( \ell \lambda_i > 0 \), we then select as a hypothesis space the \( \ell \)-dimensional subspace \( \mathcal{H}_\ell \subseteq \mathcal{B} \), where

\[
\mathcal{H}_\ell = \text{span}\{\psi_1, \ldots, \psi_\ell\}.
\]

It follows from orthonormality of the \( \phi_i \) that the \( \psi_i \) form an orthonormal set in \( \mathcal{B} \), i.e., \( \langle \psi_i, \psi_j \rangle_\mathcal{B} = \delta_{ij} \). Here, \( \cdot, \cdot \rangle_\mathcal{B} \) is the inner product of \( \mathcal{B} \), taken conjugate-linear in its first argument.

With these definitions, it follows that \( \mathcal{P}_{\mathcal{H}_\ell} \), the orthogonal projection operator onto \( \text{span}\{\psi_1, \ldots, \psi_\ell\} \). As for the inverse \((\mathcal{I}_{\mathcal{P}_{\mathcal{H}_\ell}})^{-1}\), it acts as

\[
(\mathcal{I}_{\mathcal{P}_{\mathcal{H}_\ell}})^{-1} \phi_i = (\mathcal{I}_{\mathcal{P}_{\mathcal{H}_\ell}})^{-1} u^* \phi_i / \lambda_i = \psi_i / \lambda_i^{1/2}
\]

on each eigenfunction \( \phi_i \) corresponding to a nonzero eigenvalue \( \lambda_i \). Consequently, by expanding \( Z_r \in L^2(\rho_X) \) as \( Z_r = \sum_{i=1}^r \alpha_i(\tau) \phi_i \), where

\[
\alpha_i(\tau) = \langle \phi_i \circ X, U_i Y \rangle_{L^2(\rho)}
\]

the target function \( f_{\tau,\ell} \) associated with \( \mathcal{H}_\ell \) is given by

\[
f_{\tau,\ell} = T_{\ell} Z_r = \sum_{i=1}^\ell \alpha_i(\tau) \lambda_i^{-1/2} \psi_i
\]

where \( T_{\ell} : L^2(\rho_X) \rightarrow \mathcal{H}_\ell \) is the pseudoinverse operator from (7).

Considering now the image \( \mathcal{B} = \mathcal{I}_{\mathcal{P}_{\mathcal{H}_\ell}} \) of the ambient Hilbert space under \( L^2(\rho_X) \) inclusion, one can verify that it can be characterized as the subspace

\[
\mathcal{B} = \left\{ \sum_{i=1}^\ell c_i \phi_i \in L^2(\rho_X) : \sum_{i=1}^\ell |c_i|^2 / \lambda_i < \infty \right\}.
\]

It can also be verified that \( \tilde{T} : \mathcal{B} \rightarrow \mathcal{B} \), with \( \tilde{T}(\sum_{i=1}^\ell c_i \phi_i) = \sum_{i=1}^\ell c_i \phi_i / \lambda_i^{1/2} \), is a closed-range operator whose pseudoinverse is equal to \( \ell \). That is, \( \tilde{T} \) maps each \( L^2(\rho_X) \) equivalence class in \( \mathcal{B} \) to a representative in \( \mathcal{B} \). Note that \( \tilde{T} \) is necessarily an unbounded operator if \( \mathcal{B} \) is infinite-dimensional, and, moreover, if \( G \) is strictly positive-definite (so that all \( \lambda_i \) are strictly positive), then \( \mathcal{B} \) is a proper, dense subspace of \( L^2(\rho_X) \).

In fact, \( \tilde{T} \) is closely related to the Nyström extension operator employed in applications such as function interpolation and kriging [e.g., 41]. Noticing from (12) that \( T_{\ell} = T_{\ell,\ell} \), we may therefore interpret the target function \( f_{\tau,\ell} \) as a spectrally truncated Nyström extension of \( Z_r \), which is well defined even if \( Z_r \) does not lie in \( \mathcal{B} \).

2.3. Reproducing kernel Hilbert spaces

For the remainder of the paper, we will restrict attention to the case that the response variable \( Y \) is complex-valued, i.e., \( Y = \mathbb{C} \). In this setting, the ambient Hilbert space \( \mathcal{B} \) naturally acquires the structure of an RKHS, as we describe below.

Basic properties of RKHSs. For each point \( x \in X \), let \( L_x : \mathcal{B} \rightarrow \mathbb{C} \) be the evaluation functional on the ambient Hilbert space, defined by \( L_x f = f(x) \). The space \( \mathcal{B} \) is said to be an RKHS if \( L_x \) is bounded, and therefore continuous, at every \( x \in X \). It is a known fact that no unbounded linear functional on a Banach space can be constructed without the axiom choice. Therefore, all explicitly constructible Hilbert spaces of complex-valued functions are necessarily RKHSs. Consequently, all explicitly representable target functions \( f_{\tau,\ell} \) from (7) necessarily lie in an RKHS. Note that by boundedness of \( L_x \) at every \( x \in X \), convergence of two functions in RKHS norm implies pointwise convergence on \( X \).

It follows from the Riesz representation theorem that for every \( x \in X \) there exists some function \( k_x \in \mathcal{B} \) such that

\[
f(x) = L_x f = \langle k_x, f \rangle_{\mathcal{B}}, \quad \forall f \in \mathcal{B}.
\]

The above is known as the reproducing property of \( \mathcal{B} \). The reproducing kernel \( k : X \times X \rightarrow \mathbb{C} \) of \( \mathcal{B} \) is then defined as the bivariate function

\[
k(x_1, x_2) = \langle k_{x_1}, k_{x_2} \rangle_{\mathcal{B}}.
\]

It follows from the defining properties of inner products that \( k \) is (i) conjugate-symmetric, i.e., \( k(x_1, x_2) = k(x_2, x_1)^* \) for all \( x_1, x_2 \in X \); and (ii) positive-definite, i.e., for all \( x_1, \ldots, x_m \in X \) and \( a_1, \ldots, a_m \in \mathbb{C} \),

\[
\sum_{i=1}^m a_i^* a_j k(x_i, x_j) \geq 0.
\]

Conversely, the Moore-Aronszajn theorem [42] states that for any conjugate-symmetric, positive-definite kernel function \( k : X \times X \rightarrow \mathbb{C} \), there exists a unique RKHS on \( X \) for which \( k \) is the reproducing kernel. Thus, there is a one-to-one correspondence between kernels and RKHSs. The kernel \( k \) is said to be strictly positive-definite if the inequality in (13) is strict whenever the \( x_i \) are all distinct and at least one of the \( a_i \) is nonzero.
Let \( \nu : \Sigma_X \to [0, \infty] \) be any measure such that there exists a compact embedding \( \iota \) of the RKHS \( \mathcal{B} \) into \( L^2(\nu) \). The practical utility of RKHSs manifests in the adjoint \( \iota^* : L^2(X) \to \mathcal{B} \) being representable in terms of the kernel as

\[
\iota^*_g(x) = \langle \iota \iota^*_g, g \rangle_{L^2(\nu)} = \int_X k(x, \cdot) g \, d\nu,
\]

where \( g \) is any element of \( L^2(\nu) \). Thus, the adjoint of the embedding of the RKHS \( \mathcal{B} \) into \( L^2(\nu) \) is a compact integral operator on the latter space. Similarly, \( G \) is a strictly-positive operator. In that case, \( B_G := \iota_{\iota^*} \mathcal{B} \) is a dense subspace of \( L^2(\nu) \). The kernel \( k \) will be said to be \( L^2(\nu) \)-Markov if \( G \) is a Markov operator, i.e., (i) \( \int_X G_h d\nu = \int_X h d\nu \) for all \( h \in L^2(\nu) \); and (ii) \( G_h = h \) if \( h \) is constant. It follows from these properties that the leading largest eigenvalue of \( G \) associated with a Markov kernel is equal to 1, and the corresponding eigenspace contains constant functions. An \( L^2(\nu) \)-Markov kernel is said to be ergodic if the eigenvalue at 1 is simple.

In the case \( \nu = \rho_X \), we will abbreviate \( \rho_{\mathcal{B}} = \iota \) and \( G_{\rho_{\mathcal{B}}} = G \) as in Section 2.3. The evaluation of the target function from (7) at a point \( x \in X \) is then expressible as

\[
f_{x,t}(x) = \sum_{i=1}^{\ell} \frac{\alpha_i(\tau)}{\lambda_i} (k_i, \psi_i)_{L^2(\rho_X)} = \sum_{i=1}^{\ell} \frac{\alpha_i(\tau)}{\lambda_i^{1/2}} \psi_i(x). \tag{16}
\]

Topological framework and Mercer kernels. Henceforth, we will assume that \( X \) has the structure of a metric space, equipped with its Borel \( \sigma \)-algebra \( \Sigma_X \) and \( \rho_X \) is a Borel probability measure with compact support \( X^*_\rho \subseteq X \). Given any subset \( S \subseteq X \), we will use the notation \( \mathcal{B}(S) \) to represent the RKHS on \( S \) with reproducing kernel \( k_{S \times S} \). Note that \( \mathcal{B}(S) \) embeds naturally and isometrically into \( \mathcal{B} \), so we may view it as a subspace of the latter space. We also let \( C(S) \) be the space of complex-valued continuous functions on \( S \), and \( C_b(S) \) the Banach space of bounded functions in \( C(S) \), equipped with the uniform norm. Note that \( C(S) = C_b(S) \) if \( S \) is compact.

In this setting, continuous kernel functions on \( X \), also known as Mercer kernels, have the property that their associated RKHS is a subset of \( C(X) \) \cite{11}. Moreover, for any compact set \( S \subseteq X \), the embedding \( \mathcal{B}(S) \hookrightarrow C(S) \) is bounded. If, in addition, \( S \) is the support \( X^*_\rho \) of a finite Borel measure \( \nu \) on \( X \), \( C(X^*_\rho) \) embeds into \( L^2(\nu) \) via a bounded linear map, and thus \( \iota : \mathcal{B}(X^*_\rho) \to L^2(\nu) \) is a bounded, injective operator. It also follows by continuity of \( k \) and compactness of \( X^*_\rho \) that \( G_{\nu} = \iota_{\iota^*} \) is a trace-class (and therefore compact) operator, with trace norm equal to \( \tr G_{\nu} = \int f_k(x, x') \, d\nu(x') \) \cite{12}. In particular, the compactness of \( G_{\nu} \) is equivalent to \( \iota_{\iota^*} \) being compact. Mercer’s theorem also states that for any \( x, x' \in X \), the kernel \( k(x, x') \) can be expressed through the series expansion,

\[
k(x, x') = \sum_{\ell, \lambda > 0} \psi_i(x) \psi_i(x'),
\]

where the \( \psi_i \) are orthonormal functions in \( \mathcal{B} \) associated with eigenvalue \( \lambda_i \) of \( G_{\nu} \), defined analogously to \( \| \psi_i \|_{\mathcal{B}} \), and convergence of the sum over \( i \) is uniform on \( X \times X \). This result then implies that the restrictions of the \( \psi_i \) on \( X \) form an orthonormal basis of \( \mathcal{B}(X) \) (as opposed to merely an orthonormal set). It can also be shown that every strictly positive-definite Mercer kernel is \( L^2(\nu) \)-strictly positive for any compactly supported, finite Borel measure \( \nu \).

By virtue of the above properties, Mercer kernels provide a convenient practical means of generating hypothesis spaces that are compactly embeddable into \( L^2(\rho_X) \), as required for the hypothesis spaces in Section 2.2. Note that the target function in (14) associated with a Mercer kernel is an RKHS (and thus continuous) function defined on the whole of \( X \), but its behavior outside of the support \( X^*_\rho \) makes no contribution to the excess generalization error from (5) determined through the \( L^2(\rho_X) \) norm.

2.4. Data-driven target function

We are now ready to construct the empirical target function employed in KAF. In this construction we consider a standard supervised learning scenario, where we have access to a training dataset consisting of pairs \( (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n) \), where \( x_j = X(\omega_j) \) and \( y_j = U_j Y(\omega_j) \) are the values of the covariate and response variables, respectively, on an (unknown) collection of points \( \omega_1, \ldots, \omega_n \) on the state space \( \Omega \). In practical applications, the pairs \( (x_j, y_j) \) may be obtained from a single dynamical trajectory

\[
\omega_j = A_{t_j}(\omega_0), \quad t_j = (j - 1) \Delta t, \tag{17}
\]

at a fixed sampling interval \( \Delta t > 0 \). Alternatively, the \( (x_j, y_j) \) may be generated by an ensemble of (shorter) trajectories on \( \Omega \).

Associated with every such dataset is an empirical probability measure \( \rho_{\mathcal{X}} : \mathcal{F} \to [0, 1] \), defined as \( \rho_{\mathcal{X}} = \sum_{j=1}^{n} \delta_{\omega_j} / n \), where \( \delta_{\omega_j} \) is the Dirac \( \delta \)-measure supported on \( \{\omega_j\} \subseteq \Omega \). Similarly, the empirical probability measure \( \rho_{\mathcal{X},t} : \Sigma_X \to [0, 1] \) is defined as \( \rho_{\mathcal{X},t} = \sum_{j=1}^{n} \delta_{x_j} / n \).
Intuitively, we view \( \rho_n \) and \( \rho_{X,n} \) as empirical approximations to \( \rho \) and \( \rho_X \), respectively; a connection which will be made precise in Section 3.

Next, as empirical analogs of \( L^2(\rho) \) and \( L^2(\rho_X) \), we employ the Hilbert spaces \( L^2(\rho_n) \) and \( L^2(\rho_{X,n}) \), consisting of equivalence classes of complex-valued, measurable functions on \( \Omega \) and \( X \) having common values at the sampled points \( \omega_j \) and \( x_j \), respectively. As Hilbert spaces, \( L^2(\rho_n) \) and \( L^2(\rho_{X,n}) \) have dimension at most \( n \) (with equality if all \( \omega_j \) and \( x_j \) are distinct, respectively), and can be homomorphically embedded into \( \mathbb{C}^n \), equipped with the normalized dot product \( g \cdot h/n \). That is, for every measurable function \( g : \Omega \to \mathbb{C} \), the corresponding \( L^2(\rho_n) \) equivalence class can be represented by a column vector \( g \in L^2(\rho_n) \) with \( g = [g(\omega_1), \ldots, g(\omega_n)]^T \), storing in its components the values of \( g \) on \( \omega_j \). Elements of \( L^2(\rho_{X,n}) \) are represented by \( \mathbb{C}^n \) vectors in a similar manner, while operators on \( L^2(\rho_n) \) and \( L^2(\rho_{X,n}) \) are represented by \( n \times n \) complex matrices.

Hereafter, we will refer to the \( \mathbb{C}^n \) vector
\[
y_{\tau} = [U_1 Y(\omega_1), \ldots, U_n Y(\omega_n)]^T, \tag{16}
\]
representing the \( L^2(\rho_n) \) equivalence class of the response function \( U_\tau Y \), as the analog vector. It should be noted that, in general, the dynamical flow \( A_\tau \) does not preserve null sets with respect to \( \rho_n \), and thus \( U_\tau \) does not extend to an operator on \( L^2(\rho_n) \) analogously to the Koopman operator on \( L^2(\rho) \). This means that the analog vector \( y_{\tau} \), \( \tau > 0 \), cannot be expressed as the result of applying a Koopman operator to \( y_0 \). Nevertheless, for data sampled on a single dynamical trajectory as in (15) and lead times \( \tau = q \Delta t, \) \( q \in \mathbb{N} \), an analog of the Koopman operator on \( L^2(\rho_n) \) is provided by the \( q \)-step shift operator on time series (14).

With these definitions, the empirical generalization error \( \mathcal{E}_{\tau,n} : L^2(\rho_{X,n}) \to \mathbb{R} \) is given by (cf. (4))
\[
\mathcal{E}_{\tau,n}(f) := \|f_\tau \circ X - U_\tau Y\|_{L^2(\rho_n)}^2,
\]
where \( f_\tau : L^2(\rho_n) \to L^2(\rho_n) \) maps each function in \( L^2(\rho_n) \) to its \( L^2(\rho_n) \) equivalence class. This functional is minimized by a unique element \( Z_{\tau,n} \in L^2(\rho_{X,n}) \) analogous to the regression function \( Z_{\tau} \) from Sections 2.1 and 2.3. Moreover, we may split the empirical generalization error as
\[
\mathcal{E}_{\tau,n}(f) = \mathcal{A}_{\tau,n}(f) + \sigma_{\tau,n},
\]
with (cf. (5))
\[
\mathcal{A}_{\tau,n}(f) = \|f_\tau \circ Z_{\tau,n}\|_{L^2(\rho_{X,n})}^2, \quad \sigma_{\tau,n} = \|Z_{\tau,n} \circ X - U_\tau Y\|_{L^2(\rho_n)}^2.
\]
To construct an empirical target function, we proceed again analogously to the infinite-dimensional case in Sections 2.1 and 2.3. That is, we seek the minimizer of the empirical excess generalization error \( \mathcal{A}_{\tau,n}(f) \) for \( f \) lying in an \( \ell \)-dimensional empirical hypothesis space \( \mathcal{H}_{\ell,n} \), which is chosen as a subspace of an ambient RKHS \( \mathcal{B}_n \subset C(X) \) associated with an empirical Mercer kernel \( k_{\rho} : X \times X \to \mathbb{C} \). Note that we allow the reproducing kernel \( k_{\rho} \) to depend on \( n \) in order to be able to take advantage of the variety of normalized kernel algorithms in the literature (45-48). Given any \( x \in X \), we shall refer to the \( \mathbb{C}^n \) vector
\[
k(x) = [k_\rho(x, x_1), \ldots, k_\rho(x, x_n)]^T,
\]
representing the \( L^2(\rho_{X,n}) \) equivalence class \( k_\rho(x, \cdot) \) of the kernel section \( k_\rho(x, \cdot) \in \mathcal{B}_n \) as the kernel vector. Next, because \( \mathcal{B}_n \subseteq L^2(\rho_{X,n}) \), we can consider \( t_n : \mathcal{B}_n \to L^2(\rho_{X,n}) \) as a (finite-rank, and thus compact) operator between Hilbert spaces, inducing the self-adjoint integral operator \( G_n := G_{\rho_{X,n}} = t_n^* t_n \) on \( L^2(\rho_{X,n}) \). The leading \( \ell \) orthonormal eigenvectors \( \phi_{1,n}, \ldots, \phi_{\ell,n} \) of \( G_n \), corresponding to positive eigenvalues \( \lambda_{1,n} \geq \cdots \geq \lambda_{\ell,n} \), respectively, define the \( \ell \)-dimensional empirical hypothesis space \( \mathcal{H}_{\ell,n} \subseteq \mathcal{B}_n \) given by (cf. (10))
\[
\mathcal{H}_{\ell,n} = \text{span}\{\psi_{1,n}, \ldots, \psi_{\ell,n}\},
\]
where
\[
\psi_{i,n} = t_n^* \phi_{i,n}/\lambda_{i,n}^{1/2}, \tag{17}
\]
are orthonormal functions in \( \mathcal{B}_n \). The KAF target function \( f_{T_\ell,n} \in \mathcal{H}_{\ell,n} \) is then obtained by minimizing \( \mathcal{A}_{\tau,n}(f) \) over this hypothesis space, leading, in direct analogy to (14), to
\[
f_{T_\ell,n}(x) = T_{\ell,n} Z_{\tau,n} = \sum_{i=1}^{\ell} \alpha_{i,n}(\tau) \langle \psi_{i,n}, \phi_{i,n} \rangle_{L^2(\rho_{X,n})} \psi_{i,n}(x), \tag{18}
\]
where \( \alpha_{i,n}(\tau) = \langle \psi_{i,n}, U_\tau Y \rangle_{L^2(\rho_{X,n})} \) and \( T_{\ell,n} : L^2(\rho_{X,n}) \to \mathcal{H}_{\ell,n} \) is the pseudoinverse operator associated with \( \mathcal{H}_{\ell,n} \).

The expression in (15) can be written more compactly in matrix form using the column vector representations \( \phi_i \in \mathbb{C}^n \) of the \( \phi_{i,n} \), given by eigenvectors of the \( n \times n \) kernel matrix \( G = [k_\rho(x_i, x_j)]/n \) representing \( G_n \), and chosen such that \( \phi_i \cdot \phi_i/n = \delta_{i,j} \). Note, in particular, that the expansion coefficients \( \alpha_{i,n}(\tau) \) are simply equal to the dot products \( \alpha_{i,n}(\tau) = \phi_i \cdot f_\tau/n \) with the analog vector. Treating the remaining terms in (18) in a similar manner, we arrive at the expression
\[
f_{T_\ell,n}(x) = k(x)^T A_\ell y_\tau, \quad A_\ell = \Phi_\ell A^{-1}_\ell \Phi_\ell/n^2, \tag{19}
\]
where $k(x)$ is the kernel vector, $\Phi_T$ is the $n \times \ell$ matrix whose columns consist of the eigenvectors $\phi_i \in \mathbb{C}^n$, $\Lambda_T$ is the $\ell \times \ell$ diagonal matrix whose diagonal entries consist of $\lambda_i$, and $\ast$ denotes complex-conjugate transpose. This formula expresses the KAF target function as a sesquilinear form $(k(x), y_t)$ $\mapsto$ $k(x)\ast A_T y_t$, mapping pairs of kernel and analog vectors to $\mathbb{C}$-valued forecasts. Letting $V_T = \Lambda_T^{-1/2} \Phi_T^\ast/n$, where $V_T^\ast V_T = A_T$, the empirical target function is reexpressed as

$$f_{\tau,\ell,0}(x) = V_T k(x) \cdot V_T y_t.$$ 

This particular form emphasizes that the forecast is the result of taking the inner product of suitably projected kernel vector and equivalently projected analog vectors.

### 3. Error analysis and convergence

The previous section has shown how to calculate both an empirical target function $f_{\tau,\ell,0}$ and an ideal target function $f_{\tau,\ell}$, corresponding to two different hypothesis spaces, $\mathcal{H}_{\ell,\ell}$ and $\mathcal{H}_\ell$, as well as two different error functionals, $E_{\tau,\ell}$ and $E_\tau$, respectively. This section addresses the connection between the two functions, with the ultimate goal being that of bounding the error $E_{\tau}(f_{\tau,\ell,0})$ of the empirical target function as much as possible. Among other reasons, the availability of such bounds is useful for assessing the risk of overfitting the training data; that is, the possibility that $E_{\tau}(f_{\tau,\ell,0}) \gg E_\tau(f_{\tau,\ell,0})$ for the chosen empirical hypothesis space. Note, in particular, that for a variety of kernels (e.g., strictly positive-definite kernels) it is possible to make $E_{\tau,\ell}(f_{\tau,\ell,0})$ at fixed $\ell$ arbitrarily small by increasing $\ell$, but this reduction of empirical error eventually leads to an increase of the “true” error $E_{\tau}(f_{\tau,\ell,0})$ with respect to the invariant measure of the dynamics. See Section 6.1 for an illustration of this phenomenon.

The analysis of the error $E_{\tau}(f_{\tau,\ell,0})$ is typically organized into analysis of the error $E_{\tau}(f_{\tau,\ell})$ of the ideal target function (i.e., the generalization error), and the difference in error $E_{\tau}(f_{\tau,\ell,0}) - E_{\tau}(f_{\tau,\ell})$, denoted by $D_{\tau,\ell,0}$, between the empirical and ideal target functions, referred to as the sample error [25]. In other words, error analysis uses the following decomposition:

$$E_{\tau}(f_{\tau,\ell,0}) = E_{\tau}(f_{\tau,\ell}) + D_{\tau,\ell,0} = E_{\tau}(f_{\tau,\ell}) + |E_{\tau}(f_{\tau,\ell,0}) - E_{\tau}(f_{\tau,\ell})|.$$ 

This section examines in detail these contributions, and establishes sufficient conditions for convergence of the KAF target function to the conditional expectation.

#### 3.1. KAF generalization error

The excess generalization error $\mathcal{A}_{\tau}(f_{\tau,\ell})$ from (8) of the KAF target function $f_{\tau,\ell}$ in (14) is given by

$$\mathcal{A}_{\tau}(f_{\tau,\ell}) = \|P_{H_T} Z_t\|^2_{L^2(\rho_X)} = \sum_{i=1}^{\infty} \alpha_i(\tau)^2,$$ 

where $P_{H_T} : L^2(\rho_X) \to L^2(\rho_X)$ is the orthogonal projection mapping into the orthogonal complement $H_T^\perp$ of the hypothesis space $H_T$ in $L^2(\rho_X)$. It follows from the above that $\mathcal{A}_{\tau}(f_{\tau,\ell})$ vanishes as $\ell \to \infty$ for any $Z_t \in L^2(\rho_X)$, and thus for any response variable $U_t, Y_t \in L^2(\rho)$, iff the sequence of projections $P_{H_T}$ converges pointwise to 0 as $\ell \to \infty$ (i.e., $P_{H_T} g \to 0$ for any $g \in L^2(\rho_X)$). Because $[\phi_i]_{i=1}^\infty$ is an orthonormal basis of $L^2(\rho_X)$, this happens in turn iff $G$ is a strictly positive operator. Since $\mathcal{A}_{\tau}(f) = 0$ iff $f = Z_t$, we obtain the following basic consistency result expressed in terms of a positivity condition on the kernel $k$.

**Theorem 1.** Let $k : X \times X \to \mathbb{C}$ be an $L^2(\rho_X)$-strictly-positive kernel with corresponding RKHS $\mathcal{B}$. Then, for any response variable $U_t, Y_t \in L^2(\rho)$ and lead time $\tau \geq 0$, as $\ell \to \infty$, the target functions $f_{\tau,\ell}$ from (14) converge to the conditional expectation $\mathbb{E}[U_t | Y_t] = X \ast Z_t$, in the sense that $\lim_{\ell \to \infty} \|f_{\tau,\ell} - Z_t\|^2_{L^2(\rho_X)} = 0$.

Convergence with respect to the (stronger) RKHS norm of $\mathcal{B}$, as well as more precise estimates of the $L^2(\rho_X)$ error can be obtained under the additional assumption that the regression function $Z_t$ lies in the subspace $B \subset L^2(\rho_X)$. In that case, $Z_t$ has a representative $f_{\tau} \in \mathcal{B}$, given by Nyström extension as

$$f_{\tau} = \tilde{T} Z_t = \sum_{i=1}^{\infty} \alpha_i(\tau) \phi_i / \lambda_i^{1/2},$$ 

where the infinite sum in the right-hand side converges in $\mathcal{B}$ norm. That is, $f_{\tau}$ is given by the $\mathcal{B}$-norm limit of the partial sums $\sum_{i=1}^{N} \alpha_i(\tau) \phi_i / \lambda_i^{1/2}$. The latter are precisely equal to the target functions $f_{\tau,\ell}$ from (14), and therefore we conclude that $\lim_{\ell \to \infty} \|f_{\tau,\ell} - f_{\tau}\|_{B^*} = 0$.

To obtain an estimate of $\mathcal{A}_{\tau}(f_{\tau,\ell})$, observe that $B$ coincides with the range of $G^{1/2}$, the square root of $G$. It then follows that for $Z_t \in B$, there exists $W_t \in L^2(\rho_X)$ such that $Z_t = G^{1/2} W_t$, which allows the excess generalization error to be rewritten as

$$\mathcal{A}_{\tau}(f_{\tau,\ell}) = \sum_{i=1}^{\infty} A_i (\phi_i, W_t)_{L^2(\rho_X)}^2.$$ 

The Cauchy-Schwarz inequality then yields

$$\mathcal{A}_{\tau}(f_{\tau,\ell}) \leq \left( \sum_{i=1}^{\infty} A_i \right) \|W_t\|^2_{L^2(\rho_X)}.$$ 


where $\sum_{i=1}^{\infty} \lambda_i < \text{tr} G$ is finite. Thus, in this case we can bound the decay of the excess generalization error by the decay of the tail sum of the eigenvalues of $G$.

The study of decay rates of the eigenvalues of an integral operator is a classic and still active field of research [49]. In the setting of Mercer kernels and compactly supported probability measures studied here, it can be shown that $\lambda_i = o(i^{-1})$ for large-enough $i$ [50] Theorem 2.4], which is consistent with the fact that $G$ is trace-class. Estimates of the rate of decay of the tail sum are possible under additional regularity conditions on the kernel, including, for example, specialized notions of Lipschitz continuity. In such cases, it is possible to express the decay rate of $A_i(f_{x,\ell})$ as being algebraic, i.e., $A_i(f_{x,\ell}) \leq C i^{-\gamma}$ for some positive constants $C$ and $\gamma$ [51].

3.2. KAF sample error

In this section, we will establish that, under natural assumptions on the dynamical system and the reproducing kernels, the difference in error $\Delta_{t,\ell,n}$ between the empirical and ideal target functions vanishes in the limit of large data, $n \to \infty$. We will do so by establishing a stronger result, namely that $f_{t,\ell,n}$ converges uniformly to $f_{t,\ell}$ in an appropriate compact set containing the supports of $\rho_X$ and the sampling measures $\rho_{X,n}$.

Basic assumptions for convergence. Our first assumption is that (i) $\Omega$ has the structure of a metric space, equipped with its Borel $\sigma$-algebra $\mathcal{F}$; (ii) $\rho$ is a Borel probability measure with compact support $\rho_{\Omega} \subseteq \Omega$; and (iii) all of $A_i$, $X$, and $Y$ are continuous. Note that, by continuity of $A_i$, the Koopman operator $U_i$ maps continuous functions to continuous functions for all $i \geq 0$, preserving the $C(\Omega)$ norm of bounded continuous functions.

Our second assumption pertains to the convergence of the empirical measures $\rho_n$ underlying the data to the invariant measure. Specifically, we assume that, for the starting state $\omega_1 \in \Omega$, the measures $\rho_n$ converge to $\rho$ weakly: that is, for every bounded, continuous function $g : \Omega \to C$, $\lim_{n \to \infty} \int_{\Omega} g \, dp_n = \int_{\Omega} g \, dp$. The weak convergence of $\rho_n$ to $\rho$, in conjunction with the continuity of $X$, implies in turn that $\rho_{X,n}$ converges weakly to $\rho_X$, i.e., $\lim_{n \to \infty} \int_{X} f \, dp_{X,n} = \int_{X} f \, dp_X$, for all $f \in C_b(X)$.

Our third assumption relates to the existence of a compact set in which both the the covariate data $x_i$ and the support $\rho_X$ lie. Specifically, for the starting state $\omega_1 \in \Omega$ underlying the covariate training data, we assume that there exists a compact set $\mathcal{U} \subseteq X$ containing $X_{\bar{x}} = \text{supp} \rho_X$, as well as $\text{supp} \rho_{X,n} = [x_1, \ldots, x_n]$ for every $n \in \mathbb{N}$. This condition is automatically satisfied if the state space $\Omega$ is already a compact space (e.g., ergodic dynamics on a torus), and is also satisfied by many systems with appropriate dissipative dynamics. Examples of such systems include ordinary differential equation models on $\Omega = \mathbb{R}^d$ with quadratic nonlinearities, such as the L63 system [52] studied in Section 6.2 below, as well as partial differential equation models possessing inertial manifolds [53]. For our purposes, the existence of the compact set $\mathcal{U}$ allows the (generally distinct) ideal and empirical RKHSs, $\mathcal{B}(\mathcal{U})$ and $\mathcal{B}_n(\mathcal{U})$, respectively, to be viewed as subspaces of the Banach space $C(\mathcal{U})$. In the latter space, the relevant notion of convergence is convergence with respect to the uniform norm.

Next, we make an assumption on the convergence of the empirical reproducing kernels $k_{\omega}$ in $\mathcal{B}_n$ to the reproducing kernel $k$ of $\mathcal{B}$. Specifically, we assume that, as $n \to \infty$, $k_{\omega}$ converges to $k$ uniformly on $\mathcal{U} \times \mathcal{U}$ (i.e., with respect to $C(\mathcal{U} \times \mathcal{U})$ norm). This assumption is trivially satisfied if one works with data-independent kernels, $k_n = k$, and also holds for many classes of normalized kernels, including [45–48].

Finally, we assume that the response variable $U_i Y$ is bounded on $X^{-1}(\mathcal{U})$, i.e., $C_Y = \sup_{x \in X^{-1}(\mathcal{U})}\|U_i Y(x)\| < \infty$.

Physical measures. We define the basin of $\rho$ as the maximal set $M_\rho \subseteq \Omega$ for which the sampling measures $\rho_n$, starting from any $\omega_1 \in M_\rho$, converge weakly to $\rho$. If the dynamics is ergodic (i.e., every invariant set $S \in \mathcal{F}$ under $A_t$ for all $t \in \mathbb{R}$ has either $\rho(S) = 0$ or $\rho(S) = 1$), then $\rho$-a.e. $\omega_1 \in \Omega$ lies in $M_\rho$, and the support $\rho_{\Omega}$ lies in the topological closure of $M_\rho$. In addition, for many dynamical systems encountered in applications, $M_\rho$ can be a significantly “larger” set than $\Omega_{\rho}$. In particular, for systems possessing physical measures [54], $M_\rho$ has positive measure with respect to an ambient measure on $\Omega$ (e.g., Lebesgue measure), whereas $\Omega_{\rho}$, oftentimes, has zero ambient measure (e.g., if $\rho_{\Omega}$ is an attractor developing under dissipative dynamics). In such cases, the methods will converge from an experimentally accessible set of initial conditions that can lie outside of $\Omega_{\rho}$.

Uniform convergence on $\mathcal{U}$. We assume throughout that the basic assumptions stated above hold. For simplicity, we will assume that for the given hypothesis space dimension $t$, all eigenvalues $\lambda_1, \ldots, \lambda_t$ are simple (if this is not the case, the argument presented below can be modified using appropriate projector operators onto eigenspaces of $G$ and $G_n$). We will also consider that all of the $\phi_{i,n}$, $\psi_{j,n}$, $\phi_{i}$, and $\psi_{j}$ are real, again for simplicity.
Since the ideal target function \( f_{\tau,\ell} \) from (14) and the empirical target function (18) are linear combinations of \( \ell < \infty \) continuous functions, \( \psi_i \) and \( \psi_{i,n} \), respectively, the ideal target function \( f_{\tau,\ell} \) to \( f_{\ell} \) in \( C(U) \) norm will follow if it can be shown that, as \( n \to \infty \) and for each \( i \in \{1, \ldots, \ell\} \), (i) the eigenvalues \( \lambda_{i,n} \) converge to \( \lambda_i \); (ii) the RKHS functions \( \psi_{i,n} \) converge, up to multiplication by a constant phase factor, to \( \psi_i \) in \( C(U) \) norm; and (iii) each of the expansion coefficients \( c_{i,n}(\tau) \) converges to \( c_i(\tau) \).

The first two of these claims are a consequence of the following lemma, which is based on [46] Theorem 15, [55] Corollary 2, and [56] Theorem 7.

**Lemma 2.** Under the basic assumptions for convergence, the following hold:

(i) For each nonzero eigenvalue \( \lambda_i \) of \( G \), \( \lambda_{i,n} \) converges to \( \lambda_i \) as \( n \to \infty \).

(ii) For every RKHS function \( \psi_i \) corresponding to \( \lambda_i > 0 \), there exist complex numbers \( c_{i,n} \) of unit modulus, such that \( \|\psi_{i,n} - c_{i,n}\psi_i\|_{C(U)} = 0 \).

Next, let \( T_n : B_n \to B_n \) be the empirical Nyström extension operator on \( B_n := \psi_i B_n \), defined analogously to \( T \) from Section 2.2. Also, for any probability measure \( \nu : \mathcal{F} \to [0,1] \), let \( \nu(f) = \int f \, d\nu \); where \( f \in L^1(\nu) \). To verify convergence of the expansion coefficients \( \alpha_{i,n}(\tau) \), note that Lemma 2(ii) implies that for each \( i \) such that \( \lambda_i > 0 \), the continuous representatives of \( \psi_{i,n} \) given by \( \varphi_{i,n} = T_n \varphi_i = \psi_{i,n} \phi_{i,n}^{1/2} \), converge in \( C(U) \) norm and up to phase to the continuous representative \( \varphi_i = T \varphi_i = \psi_i \phi_i^{1/2} \) of \( \psi_i \). Moreover, because the products \( \alpha_{i,n}(\tau) \varphi_{i,n} \) are invariant under multiplication of \( \varphi_{i,n} \) by a constant phase factor, without loss of generality, we may assume that the \( c_{i,n} \) in Lemma 2 are all equal to 1. Then, we have

\[
|\alpha_{i,n}(\tau) - \alpha_i(\tau)| = |\rho_n((\varphi_{i,n} \circ X) U, Y) - \rho((\varphi_i \circ X) U, Y)|
\]

\[
\leq |\rho_n((\varphi_{i,n} - \varphi_i) \circ X) U, Y)| + |(\rho_n - \rho)((\varphi_i \circ X) U, Y)|
\]

\[
\leq C_1 |\varphi_{i,n} - \varphi_i|_{C(U)} + |\rho_n - \rho|((\varphi_i \circ X) U, Y).
\]

In the last line above, the first term converges to 0 by uniform convergence of \( \varphi_{i,n} \) to \( \varphi_i \) on \( U \), and the second term by weak convergence of \( \rho_n \) to \( \rho \), so we conclude that \( \alpha_{i,n}(\tau) \) converges to \( \alpha_i(\tau) \). Moreover, by continuity of the dynamics and covariate and response variables, the convergence is uniform with respect to \( \tau \) lying in compact sets.

We summarize the main results of Sections 3.1 and 3.2 in the following theorem:

**Theorem 3.** Under the basic assumptions for convergence, for every lead time \( \tau \geq 0 \) and \( \ell \) such that \( \ell > 0 \), the KAF target function \( f_{\tau,\ell} \in B_c \) converges as \( n \to \infty \) to the ideal target function \( f_{\tau,\ell} \in B_c \), uniformly on \( U \). Moreover, if the reproducing kernel \( k \) is \( L^2(\rho_X) \)-strictly-positive-definite, then by Theorem 7 \( f_{\tau,\ell} \) converges to the regression function \( Z_\ell \) associated with the conditional expectation, \( \mathbb{E}[U_\tau \mid X] = Z_\ell \circ X \), in the sense of the iterated limit

\[
\lim_{\ell \to \infty} \lim_{n \to \infty} f_{\tau,\ell,n} = \lim_{\ell \to \infty} f_{\tau,\ell} = Z_\tau.
\]

Here, the \( n \to \infty \) and \( \ell \to \infty \) limits are taken in \( C(U) \) and \( L^2(\rho_X) \) norm, respectively. Moreover, the convergence is uniform with respect to \( \tau \) lying in compact sets.

### 3.3. Mixing and loss of predictability

Before closing Section 3 we discuss some aspects of the long-time behavior of the conditional expectation and the KAF target functions in the presence of mixing dynamics, which will be useful in our interpretation of the L63 experiments in Section 6.2. First, we recall that the measure-theoretic definition of mixing [e.g., 57] can be equivalently stated as the condition that for any \( g, h \in L^2(\rho) \),

\[
\lim_{\tau \to \infty} \mathbb{E}[U_\tau g \mid h]_{L^2(\rho)} = \left( \int_{\Omega} \mathbb{E}[g] \, d\rho \right) \left( \int_{\Omega} h \, d\rho \right).
\]

Thus, under mixing dynamics, inner products of the form \( \langle U_\tau g, h \rangle_{L^2(\rho)} \), which can be thought of as temporal cross-correlation functions, converge to constants equal to products of the expectation values \( \mathbb{E}[g^2] = \int_{\Omega} g^2 \, d\rho \) and \( \mathbb{E}[h] = \int_{\Omega} h \, d\rho \). Using the projection representation of the conditional expectation in (3), it then follows that

\[
\lim_{\tau \to \infty} \mathbb{E}[U_\tau Y \mid X]_{L^2(\rho)} = \lim_{\tau \to \infty} \mathbb{E}[P_{L^2(\rho)\downarrow\Omega} U_\tau Y]_{L^2(\rho)}
\]

\[
= \lim_{\tau \to \infty} \mathbb{E}[P_{L^2(\rho)\downarrow\Omega} U_\tau Y]_{L^2(\rho)}
\]

\[
= \mathbb{E}[P_{L^2(\rho)\downarrow\Omega} \mathbb{E}[Y]_{L^2(\rho)}]
\]

Therefore, because \( g \) in the above is arbitrary, and \( P_{L^2(\rho)\downarrow\Omega} \) leaves constant functions invariant, we conclude that \( \mathbb{E}[U_\tau Y \mid X] \) converges weakly to a constant function equal to \( \mathbb{E}[Y] \), i.e.,

\[
\lim_{\tau \to \infty} \mathbb{E}[U_\tau Y \mid X] - \mathbb{E}[Y]_{1\Omega}_{L^2(\rho)}
\]

\[
= \lim_{\tau \to \infty} \mathbb{E}[P_{L^2(\rho)\downarrow\Omega}(U_\tau Y - \mathbb{E}[Y]_{1\Omega})_{L^2(\rho)}] = 0,
\]

where \( 1_{\Omega} \) is the function on \( \Omega \) equal everywhere to 1.

We interpret this behavior as a loss of predictability due to mixing dynamics.
Observe now that the \( L^2(\rho) \) element \( f_{z,\ell} \circ X \), where \( f_{z,\ell} \) is the ideal target function, can be expressed as \( P_R U_i Y \), where \( P_R \) is the orthogonal projection on \( L^2(\rho) \) mapping into the pullback \( \tilde{\mathcal{H}}_R = H_1 \circ X \) of the \( \ell \)-dimensional hypothesis space \( H_1 \) into \( L^2(\rho,G) \). If \( H_1 \) contains constant functions, then it follows from similar arguments as above, in conjunction with the fact that \( \tilde{\mathcal{H}}_R \) is finite-dimensional, that as \( \tau \to \infty \), \( f_{z,\ell} \) converges in \( L^2(\rho) \) norm (and not merely weakly) to \( \mathbb{E}[Y] \). We will discuss practical ways of ensuring that \( \tilde{\mathcal{H}}_R \) always contains constant functions, ensuring in turn this type of long-term statistical consistency, using Markov-normalized reproducing kernels in Section 5.

With regards now to the empirical target function, since the \( n \to \infty \) convergence of \( f_{z,\ell,n} \) to \( f_{z,\ell} \) may not be uniform with respect to \( \tau \in \mathbb{R} \), we cannot use this result to make a statement about the relation between \( f_{z,\ell,n} \) and \( \mathbb{E}[Y] \) as \( \tau \to \infty \). Nevertheless, it is still possible to ensure (through Markov normalization of the kernel) that, at fixed \( n \), \( f_{z,\ell,n} \circ X \) lies in a finite-dimensional subspace of \( L^2(\rho) \) containing constant functions. In that case, for large-enough \( n \), and long-enough, but bounded, \( \tau \), we can expect \( f_{z,\ell,n} \) to be an approximately constant function equal to \( \mathbb{E}[Y] \).

4. Extensions

This section shows how the KAF/KPCR learning framework presented thus far can shed light on other aspects of the kernel approach other than using leading principal components (eigenfunctions) to approximate the conditional expectation of observables. The first extension describes how KRR may be characterized as resulting from the same variational problem as that of KPCR, albeit with a nonlinear, rather than linear, hypothesis space. The second extension shows how quantities other than the conditional expectation, such as the conditional probability and estimates of the forecast error, may also be approximated, and what their utility may be in practical problems.

4.1. Kernel ridge regression (KRR)

In KRR, the hypothesis space is a closed ball of radius \( R \) in the RKHS \( \mathcal{B} \):

\[
\mathcal{H}_R = \{ f \in \mathcal{B} : \| f \|_{\mathcal{B}} \leq R \}.
\]

Note that \( \mathcal{H}_R \) is not a linear subspace of \( \mathcal{B} \), and thus the projection \( P_{\mathcal{H}_R} : L^2(\rho_X) \to L^2(\rho_X) \) mapping into \( \mathcal{H}_R = \iota_{\mathcal{H}_R} \) is a nonlinear operator. Although representations for this particular nonlinear operator are known \(^{[25]}\), those for the inverse \( \iota_{\mathcal{H}_R}^{-1} \) are generally intractable.

However, by using Lagrangian multipliers, optimization over \( \mathcal{H}_R \) may be transformed into a linear problem. In particular, the problem of minimizing \( \| f - Z \|_{L^2(\rho_X)} \) such that \( \| f \|_{\mathcal{B}} \leq R \) is a constrained optimization problem for which there exists a parameter \( \eta_R > 0 \), dependent on \( R \), such that the penalized optimization problem

\[
\min_{f \in \mathcal{B}} \| f - Z \|_{L^2(\rho_X)} \quad \text{with} \quad \| f \|_{\mathcal{B}} \leq R
\]

is an equivalent formulation. The solution to this problem is known to be \(^{[25]}\)

\[
f_{z,R} = \iota^*(G + \eta_R I)^{-1} Z_R.
\]

The empirical solution \( f_{z,R,n} \in \mathcal{B}_n \), meanwhile, is given by

\[
f_{z,R,n}(x) = k(x)^T (G + \eta_R I)^{-1} y_R,
\]

where \( G, k, \) and \( y_R \) are the kernel matrix, kernel vector, and analog vector from Section 2.4. As with KPCR, the KRR target function \( f_{z,R} \) also converges in mean square to the conditional expectation, in the sense that, as the regularization parameter \( \eta_R \) is decreased to zero, \( \| f_{z,R} - Z_R \|_{L^2(\rho_X)} \) converges to zero if the kernel \( k \) is \( L^2(\rho_X) \)-strictly-positive (cf. Theorem \(^{[1]}\)). Moreover, under the assumptions stated in Section 5.2, \( f_{z,R,n} \) converges to \( f_{z,R} \) in \( C(\mathcal{H}) \) norm, as \( n \to \infty \), so that an analog of Theorem \(^{[5]}\) holds for \( f_{z,R,n} \).

KRR thus relies on a full inversion of a kernel matrix, whose eigenvalues are perturbed away from zero by some regularizing parameter \( \eta_R \), whereas KPCR relies on inversion of a low-dimensional \( \ell \)-rank approximation of the kernel matrix. Both methods approximate the conditional expectation when the parameters are sufficiently relaxed, but the rates of convergence may differ. In general, KRR is useful when insensitivity to noise is desired and overfitting is to be avoided, but it can be computationally expensive as it involves full matrix inversion. KPCR, on the other hand, can converge very rapidly when it turns out that the regression function lies in the leading eigenspaces of \( G \).

4.2. Conditional variance and conditional probability

In forecasting applications, it is important to be able to perform uncertainty quantification: that is, estimate the error of the target function. Moreover, besides point forecasts of a given response variable, it is oftentimes of interest to predict the probability of occurrence of events defined in terms of the response meeting certain criteria (e.g., exceeding a specified threshold). We now discuss how KAF techniques can be employed to carry out these tasks.
First, regarding error estimation, consider the $L^2(\rho)$ observable
\[
\beta_\tau = |U_\tau Y - \mathbb{E}[U_\tau | X]|^2,
\]
which measures the square error of the conditional expectation (and thus, the optimal target function $Z_\tau$). The conditional expectation of $\beta_\tau$ with respect to $X$ is known as the conditional variance,
\[
\text{var}[U_\tau Y | X] = \mathbb{E}[\beta_\tau | X],
\]
and satisfies
\[
\int_{\Omega} \text{var}[U_\tau Y | X] d\rho = \sigma_\tau
\]
by construction. Thus, the conditional variance is equal in expectation to the intrinsic error from (6), providing an unbiased estimator of the square forecast error. Moreover, being a conditional expectation, var[$U_\tau | X$] is expressible as the pullback of a unique $W_\tau \in L^2(\rho_X)$, such that var[$U_\tau | X$] = $W_\tau \circ X$, which can be empirically approximated using KAF. Specifically, applying KAF to the function $\beta_{\tau,\omega,n} = |U_\tau Y - f_{\tau,\omega,n} \circ X|^2$ leads to the estimator $s_{\tau,\omega,n} \in \mathcal{B}_2$, of $W_\tau$ given by
\[
s_{\tau,\omega,n}(x) = k(x)^T A_\omega \beta_{\tau,\omega,n},
\]
where $\beta_{\tau,\omega,n} = [\beta_{\tau,\omega_1}(x), \ldots, \beta_{\tau,\omega_n}(x)]^T$ is a column vector in $\mathbb{C}^n$ containing the values of $\beta_{\tau,\omega,n}$ on the training states $\omega_i$ (cf. the analog vector $y_\tau$ in (16)). Because $s_{\tau,\omega,n}(x)$ is not guaranteed to be non-negative, in practice we perform error estimation using
\[
\varepsilon_{\tau,\omega,n}(x) = [s_{\tau,\omega,n}(x)]^{1/2}. \tag{20}
\]
The function $\varepsilon_{\tau,\omega,n} \circ X$ then converges in the limit of large data to $\sqrt{\text{var}[U_\tau Y | X]}$, analogously to the convergence of $f_{\tau,\omega,n} \circ X$ to $\mathbb{E}[U_\tau Y | X]$ in Theorem 3. More generally, note that for any function $\Gamma : \mathbb{C} \to \mathbb{C}$, such that $\Gamma \circ Y$ lies in $L^2(\rho)$, the conditional expectation $\mathbb{E}[U_\tau (\Gamma \circ Y) | X]$ is approximated by
\[
g_{\tau,\omega,n}(x) = k(x)^T A_\omega \Gamma(y_\tau), \tag{21}
\]
where $\Gamma(y_\tau)$ is the column vector in $\mathbb{C}^n$ obtained by element-wise application of $\Gamma$ to the analog vector $y_\tau$.

Next, turning to approximations for conditional probability, let $S \in \mathcal{F}$ be an event (i.e., a measurable subset of $\Omega$), defined through certain conditions on $Y(\omega)$ being met. For instance, in the forecasting of rare or extreme events, one might employ a formulation such as
\[
S = \{\omega \in \Omega : Y(\omega) > \theta\}, \tag{22}
\]
where $\theta$ is a large threshold parameter.

Every event $S$ has an associated indicator function $X_S \in L^2(\rho)$, evolving under the action of the Koopman operator as
\[
U_\tau X_S = X_S, \quad S_\tau = A^{-\tau}(S).
\]
Note, in particular, that every point lying initially in $S_\tau$ will be mapped into $S$ after dynamical evolution over time $\tau$. The conditional expectation
\[
\mathbb{P}[S_\tau | X] := \mathbb{E}[U_\tau X_S | X]
\]
then gives the conditional probability for $S$ to occur at lead time $\tau$ given $X$. In the context of KAF, approximations for conditional probability are obtained by setting $\Gamma$ in (21) to be the indicator function of the set $Y(S) \subset \mathbb{C}$, leading to the target function
\[
g_{\tau,\omega,n}(x) = k(x)^T A_\omega \chi_{Y(S)}(y_\tau), \tag{23}
\]
Because $g_{\tau,\omega,n}$ is not guaranteed to take values in interval $[0, 1]$, in order to obtain meaningful forecasts of conditional probability we threshold it, leading to the estimator
\[
g_{\tau,\omega,n}(x) = \begin{cases} 1, & g_{\tau,\omega,n}(x) > 1, \\ g_{\tau,\omega,n}(x), & 0 < g_{\tau,\omega,n}(x) \leq 1, \\ 0, & g_{\tau,\omega,n}(x) \leq 0, \end{cases}
\]
where $g_{\tau,\omega,n} \circ X$ approximates $\mathbb{P}[S_\tau | X]$ analogously to Theorem 3. For example, for the event in (22), $g_{\tau,\omega,n}(x)$ estimates the likelihood that $Y$ will exceed $\theta$ at lead time $\tau$, given the covariate value $x \in X$.

5. Choice of kernel

In this section, we discuss practical guidelines for choosing the kernel $k_\omega$ on covariate space $X$ employed in KAF.

5.1. Strictly positive-definite kernels

As a general guideline, in order to ensure that the method is able to converge to the regression function $Z_\tau$ for an arbitrary response variable $Y$ and lead time $\tau$ (i.e., Theorem 3 holds), the empirical kernels $k_\omega$ should converge, as $n \to \infty$, to an $L^2(\rho_X)$-strictly-positive kernel $k$, uniformly on the compact set $\mathcal{U} \subset X$. Because every Mercer kernel which is strictly positive-definite on the support of a compactly supported Borel probability measure $\nu$ is $L^2(\nu)$-strictly-positive (see Section 2.3), a convenient way of ensuring $L^2(\rho_X)$-strict-positivity of $k$ is to work with empirical kernels $k_\omega$ whose restrictions
on supp ρ_{x,a} = \{x_1, \ldots, x_n\} are strictly positive-definite for every \( n \in \mathbb{N} \). For example, in the case \( X = \mathbb{R}^d \), it is known that radial Gaussian kernels are strictly positive-definite on the whole of \( X \) [58]. Therefore, one can work with
\[
k_n(x, x') = k(x, x') = e^{-\|x-x'\|^2/\epsilon}
\] for some positive bandwidth parameter \( \epsilon \), and the conditions of Theorem 3 will be satisfied. The radial Gaussian kernel in (24) will be employed in the circle example in Section 6.1. See Ref. 59 for additional examples of kernels commonly used in machine learning applications.

It should be noted that on the finite-dimensional linear covariate space \( \mathbb{R}^d \) the covariance kernel, \( k(x, x') = x \cdot x' \), which is employed in the proper orthogonal decomposition [60] and linear inverse modeling techniques [61], is not \( L^2(\rho_X) \)-strictly-positive. Indeed, one can verify that for this choice of kernel, the corresponding integral operators \( G_n \) and \( G \) are of at most rank \( d \) [62, Section 9], thereby bounding the dimension of the hypothesis spaces \( \mathcal{H}_{\epsilon,n} \) and \( \mathcal{H} \) by \( d \). Thus, unless \( Z_G \) happens to lie in the span of the leading \( d \) eigenfunctions of \( G \) (which are, in this case, linear functions on \( X \)), the empirical target function \( f_{\epsilon,t,n} \) will fail to converge to \( Z_G \).

5.2. Variable-bandwidth, Markov kernels

Next, we discuss two modifications of the radial Gaussian kernel on \( \mathbb{R}^d \), which can play a fairly substantial role in improving the robustness of the hypothesis space, particularly for data with strong contrasts in sampling density (e.g., the L63 example in Section 6.2).

**Variable bandwidth.** Our first modification is to introduce a strictly-positive, continuous bandwidth function \( r_n : X \rightarrow \mathbb{R} \), turning (24) into a variable-bandwidth kernel, viz.
\[
k_n(x, x') = \exp\left(-\frac{{\|x-x'\|^2}}{{\epsilon r_n(x)r_n(x')}}\right)
\] (25)

Intuitively, the role of \( r_n \) is to correct for variations in the sampling density of the data in covariate space. In particular, for a well conditioned kernel integral operator \( G_n \), the number of datapoints lying within radius \( O(\epsilon^{1/2}) \) balls centered at each datapoint should not exhibit significant variations across the dataset, yet, the standard radial Gaussian kernel from (24) has no mechanism for preventing this from happening. For appropriately chosen \( r_n \), the variable-bandwidth kernel in (25) can, in effect, vary the radii of these balls to help improve conditioning. The different bandwidth functions proposed in the literature include near-neighbor distances [63] and kernel density estimates [48]. In the numerical experiments of Section 6.2, we will employ the latter approach, defining
\[
r_n(x) = q_n^{-1/m}(x),
q_n(x) = \frac{1}{(2\pi)^{d/2}} \int_X e^{-\|x-x'\|^2/\epsilon} d\rho_X(x').
\] (26)

Here, \( \epsilon \) a positive bandwidth parameter (different from \( \epsilon \) in (25)), and \( m \) a positive parameter approximating the dimension of the support \( X_G \). The parameters \( \epsilon, \tilde{\epsilon}, \) and \( m \) are all determined from the data automatically. See [36, 44] for descriptions of this procedure, including pseudocode [36, Algorithm 1].

It can be shown [50] that if \( X_G \) has the structure of a smooth manifold, with a Riemannian metric inherited from its embedding in \( X = \mathbb{R}^d \), the bandwidth functions \( r_n \) in (26) induce a conformal change of metric, such that, in the new geometry, the measure \( \rho_X \) has uniform density relative to the Riemannian measure. That is, the conformal change of metric can be thought of as “balancing out” variations of the sampling density relative to the ambient-space metric, thus improving robustness to sampling errors. It should be noted that while here we do not assume that \( X_G \) has manifold structure, the balancing effect of the bandwidth functions is still expected to take place.

**Markov normalization.** Our second modification of the radial Gaussian kernel is to normalize it to a \( L^2(\rho_X) \)-strictly-positive Markov-ergodic kernel using the normalization procedure introduced in [47]. This involves first computing the strictly positive, continuous functions
\[
u_n(x) = \int_X k_n(x, x') \, d\rho_X(x'),
\]
\[
u_n(x) = \int_X k_n(x, x') \, d\rho_X(x'),
\]
and then defining the Markov kernel \( p_n : X \times X \rightarrow \mathbb{R} \), with
\[
p_n(x, x') = \int_X k_n(x, x'') \frac{k_n(x'', x')}{u_n(x') u_n(x'')} \, d\rho_X(x'').
\] (27)

It can be readily verified that with this definition \( p_n \) acquires the Markov property, \( \int_X p_n(x, x') \, d\rho_X(x') = 1 \), for all \( x \in X \). Moreover, it can be shown that if \( k_n \) is strictly positive-definite on \( \text{supp}(\rho_X) \), then so is \( p_n \) [64, Lemma 12]. It can further be shown [55] that as \( n \to \infty \), \( p_n \) converges in \( C(\mathcal{U}) \) norm to an \( L^2(\rho_X) \)-strictly-positive Markov kernel \( p : X \times X \rightarrow \mathbb{R} \) (given
by an analogous formula to (27), so that the spectral convergence results in Lemma 2 hold with $k_n$ and $k$ replaced by $p_n$ and $p$, respectively.

Normalized kernels have previously been employed for a variety of learning applications, including spectral clustering [46] and approximation of heat operators on manifolds [45]. In the context of KAF, a useful property of Markov kernels is that the associated integral operators $G_n$ and $G$ have the top eigenvalue $\lambda_{1,n} = \lambda_1 = 1$ with a constant corresponding eigenfunction. This implies, in particular, that the corresponding RKHSs, $B_n$ and $B$, respectively, always contain constant functions, and thus can naturally capture the mean of the response variable $U_t Y$. The eigenfunctions corresponding to $< 1$ eigenvalues can then be thought of as capturing progressively finer-scale features of $U_t Y$, which are orthogonal to the mean. An illustration of this behavior is provided in Figures 2 and 3 ahead. In fact, in many ways, an ergodic, Markov reproducing kernel resembles a Sobolev space associated with a heat kernel [14]. In the context of KAF, a useful property of Markov kernels is that the associated integral operator $G$ then becomes

$$\rho(x, x') \phi(x') dx' = \lambda \phi(x).$$

A closed, analytic expression for this eigenvalue problem is not known for arbitrary choices of kernel $k$. Instead, using the radial Gaussian kernel from (24), we numerically solve the eigenvalue problem for the data-driven operator $G_n$, constructed from a sequence $x_1, \ldots, x_n \in \mathbb{R}$ of covariate points obtained from an underlying dynamical trajectory $\omega_1, \ldots, \omega_n \in S^1$, as described in Section 2.4. Using the corresponding sequence $y_{1,\ell}, \ldots, y_{n,\ell} \in \mathbb{R}$ of response variables, we then build the KAF target function $f_{r,\ell,n}$ via (18).

Here, we set the frequency $\alpha = \sqrt{2} \omega$, and employ a training dataset of $n = 1000$ samples, taken at an interval of $\Delta t = 2\pi/100$ time units. Note that $\Delta t$ is rationally independent from the rotation period, which ensures that the discrete-time map $A_n \rho$ provides an ergodic sampling of $\rho$. Using this dataset, we have computed $f_{r,\ell,n}$ for lead times $\tau = q \Delta t/\alpha$, with $q$ an integer in the interval $[0, 24]$. To assess forecast skill, one can compute the mean square error (MSE)

$$\tilde{E}_{\tau,n}(f_{r,\ell,n}) = \frac{1}{m} \sum_{j=1}^{m} (f_{r,\ell,n}(\tilde{x}_j) - U_t Y(\tilde{\omega}_j))^2$$

Under this setup, we have $U_t Y(\omega) = \sin(\omega + \alpha t)$, and the conditional expectation $\mathbb{E}[U_t Y | X = x]$ is the average of $U_t Y$ at the two angles for which $X(\omega + \alpha t) = x$; specifically,

$$Z_t(x) = \frac{\sin(\arccos(x) + \alpha t) + \sin(- \arccos(x) + \alpha t)}{2} = x \sin(\alpha t).$$

The intrinsic error $\sigma_\tau$, may then be computed directly as

$$\sigma_\tau = ||Y||_{L^2(\rho)}^2 (\alpha t)^2, \quad ||Y||_{L^2(\rho)}^2 = 1/ \sqrt{2}.$$
on a verification dataset $\tilde{\omega}_j = A_{(j-1),\Delta}(\tilde{\omega}_j)$, $\tilde{x}_j = X(\tilde{\omega}_j)$. Since the intrinsic error happens to be analytically expressible for this problem, we report the empirical excess generalization error

$$\tilde{A}_m(f_{\tau,\ell,\omega}) = \frac{1}{m} \sum_{j=1}^{m} f_{\tau,\ell,\omega}(\tilde{x}_j) - Z_{\tau}(\tilde{x}_j)^2.$$ 

The empirical MSE and excess generalization error approximate the true error $E$ and excess generalization error $\mathcal{E}_\tau(f_{\tau,\ell,\omega})$ and $\mathcal{A}_\tau(f_{\tau,\ell,\omega})$, respectively, and converge to these quantities as $m \to \infty$. Here, we employ a verification dataset of $m = 10,000$ samples, starting from a state $\tilde{\omega}_1$ chosen randomly and uniformly on the interval $[0, 2\pi]$ (so that $\omega_1 - \tilde{\omega}_1$ and $\Delta \tau$ are rationally independent with probability 1).

Figure 1 shows the absolute value of empirical excess generalization error, plotted against the bandwidth parameter $\epsilon$ of the Gaussian kernel and the hypothesis space dimension $\ell$ for representative lead times $\tau$ in the range $[0, \pi/(2\sigma)]$. In Figure 1(a), $\ell$ is kept fixed at 15, and $\epsilon$ varies logarithmically in the interval $[10^{-4}, 10^2]$. The results show agreement between several different choices of $\epsilon$ in some regimes of $\tau$, but also notable discrepancy in the region where the intrinsic error is already very small (i.e., when $\sigma \tau$ is close to $\pi/2$). In such a regime, the less sensitive kernels of large bandwidth are better able to capture that the generalization error is close to 0. In general, the $\tilde{A}_m$ values in Figure 1(a) lie approximately in the interval $[10^{-4}, 3 \times 10^{-1}]$, which corresponds to approximately $2 \times 10^{-4}$ to $5 \times 10^{-1}$ multiples of the squared $L^2(\rho)$ norm of the covariate variable.

Figure 1(b) shows the behavior of empirical excess generalization error at fixed $\epsilon = 0.1$ and representative values of $\ell$ in the range 1 to 60. Employing just the first eigenfunction performs best for $\sigma \tau = 0$, but employing more eigenfunctions is better for larger values of $\sigma \tau$. Most notable, however, is the characteristic bias-variance tradeoff as $\ell$ increases, with a valley of optimal values of $\ell$ between 10 and 30. For instance, at $\sigma \tau = 1.5$, the error decreases from $\approx 2 \times 10^{-1}$ for $\ell = 1$ to a minimal value of $\approx 2 \times 10^{-4}$ for $\ell = 20$, but then increases for larger $\ell$ to $\approx 10^{-2}$ values. This is a manifestation of the fact that the true error $\mathcal{E}_\tau(f_{\tau,\ell,\omega})$ may increase with $\ell$ at fixed $\tau$ and $n$, even though the empirical error $\mathcal{A}_m(f_{\tau,\ell,\omega})$ is always a non-increasing function of $\ell$.

6.2. Lorenz 63 system

In the L63 system $\{38\}$, the state space is $\Omega = \mathbb{R}^3$. The dynamical flow $A_{\omega_0}$ starting from $\omega_0 \in \mathbb{R}^3$ is given by solution of the initial-value problem

$$\dot{\omega}(t) = \tilde{V}(\omega(t)), \quad \omega(0) = \omega_0,$$

where $\tilde{V} : \mathbb{R}^3 \to \mathbb{R}^3$ is the smooth vector field with components $(V^1, V^2, V^3)$ at $\omega = (\omega^1, \omega^2, \omega^3)$ given by $V^1 = \sigma(\omega^2 - \omega^1)$, $V^2 = \omega^1(\rho - \omega^3)$, and $V^3 = \omega^1 \omega^2 - \beta \omega^3$. Here, $\beta$, $\rho$, and $\sigma$ are real parameters, which we set to the classical values $\beta = 8/3$, $\rho = 28$, and $\sigma = 10$. For this choice of parameters, the L63 system is rigorously known to have a compact attractor $\omega_0 \in \mathbb{R}^3$ $\{65\}$ with fractal dimension $\approx 2.06$ $\{66\}$, supporting a physical invariant measure $\mu$ with a single positive Lyapunov exponent $\Lambda \approx 0.91$ $\{67\}$. Due to dissipative dynamics, the attractor is contained within absorbing balls $\{52\}$, ensuring the existence of the compact set $\mathcal{U} \subseteq \mathbb{X}$ in covariate space. In light of these facts, all of the assumptions on the dynamical system made in Section 5.2 rigorously hold. The L63 system is also rigorously known to be mixing $\{68\}$, and thus exhibits the loss of long-term predictability discussed in Section 3.3.

In the experiments that follow, we shall let $\mathcal{Y} = \mathbb{R}$, and let the response variable $Y : \Omega \to \mathcal{Y}$ pick out one of the state vector components, i.e., if $\omega = (\omega^1, \omega^2, \omega^3) \in \mathbb{R}^3$, then $Y(\omega) = \omega^3$, for either $i = 1, 2, 3$. To illustrate the conditional probability framework discussed in Section 4.2 for each such response variable we will consider the event $S = \{\omega \in \Omega : Y(\omega) > \theta\}$, where $\theta$ is an empirical mean of $Y$ computed from the training data. That is, we will use KAF to estimate the conditional probability that the components of the state vector exceed their mean values. As for the covariate variable $X$, we will consider two cases, namely, full observations, $X = \mathbb{R}^3$ and $X = \Id$, and a partially observed setup with $X = \mathbb{R}$ and $X(\omega) = \omega^3$. Consequently, in the partially observed setup $\mathbb{E}[U | Y | X]$ represents the conditional expectation of the $i$-th component of $A_\ell(\omega)$, given the first component of $\omega$.

All experiments use covariate data $x_j = X(\omega_j)$ and response data $y_{r,j} = U_j Y(\omega_j)$ generated from the same underlying trajectory $\omega_1, \ldots, \omega_n \in \mathbb{R}^3$, with $\omega_j = A_{(j-1),\Delta}(\omega_j)$. Here, the sampling interval $\Delta$ is equal to 0.01 natural time units (i.e., about 1/100 of the characteristic Lyapunov timescale $1/\Lambda$ of the system). The trajectory $\omega_j$ was numerically generated in Matlab using the ode45 solver, starting from an arbitrary initial condition and waiting for a long spinup time before collecting the first sample $\omega_0$. We use a total of $n = 64,000$ training samples. To assess forecast skill, we use empirical root mean square error (RMSE) metrics computed from an independent verification dataset as in the circle example of Section 6.1. Specifically, the RMSE
of the target function \( f_{\tau,\ell,n} \) at lead time \( \tau \) is given by
\[
\sqrt{\mathcal{E}_{m}(f_{\tau,\ell,n})},
\]
where the verification dataset has the same number of \( m = 64,000 \) samples as the training dataset, and was obtained via a similar spinup procedure starting from a different initial condition. Note that aside from the covariate and response data in the training phase, and the covariate data in the verification phase, no other information about the system state and/or dynamics was provided to the KAF algorithm.

The first step in the KAF pipeline is to compute the kernel eigenfunctions \( \phi_{i,n} \), whose corresponding RKHS functions \( \psi_{i,n} \) form orthonormal bases for the hypothesis spaces \( \mathcal{H}_{n,\ell} \). For that, we employ the variable-bandwidth, Markov-normalized kernels from (27), with automatically tuned bandwidth and dimension parameters (see Section 5). Representative eigenfunctions for the fully- and partially-observed systems are displayed in Figures 2 and 3, respectively, in both scatterplot and time series form. There, it is evident that the eigenfunctions behave like a generalized Fourier basis on the support of the measure \( \rho_X \), with eigenfunctions corresponding to smaller eigenvalues allowing to resolve functions of increasingly smaller-scale variability on the L63 attractor. Notice, in particular, that in the partially observed example with \( X = \mathbb{R} \), the \( \phi_{i,n} \) are increasingly oscillatory, orthogonal functions on the real line, which pull back to \( G \)-measurable functions on the attractor in \( \mathbb{R}^3 \) with no variability in the \( \omega_2 \) and \( \omega_3 \) coordinates. It is precisely such a lack of variability that contributes to degraded forecast skill when faced with non-injective covariate functions.

Next, using the eigenfunctions and the response data in the training phase, we construct the empirical target functions \( f_{\tau,\ell,n} \) from (18). We also compute the error estimators \( \epsilon_{\tau,\ell,n} \) from (20), which we use to place "error bars" around our forecasts of the form \( f_{\tau,\ell,n}(x) \pm \epsilon_{\tau,\ell,n}(x) \). According to Section 4.2, for an unbiased error estimate, the RMS value of \( \epsilon_{\tau,\ell,n} \) in the verification phase should be close to the actual RMS forecast error. We use \( \ell = 3000 \) and 1000 eigenfunctions for the fully observed and partially observed setups, respectively.

Figure 4 shows prediction results for the three components of the state vector for the fully observed and partially observed systems, together with error estimates based on \( \epsilon_{\tau,\ell,n} \). We show representative forecast trajectories starting from an arbitrary initial condition in the verification condition in the verification dataset, as well as aggregate RMSE scores as a function of lead time, normalized by...
Figure 2: Representative data-driven eigenfunctions $\phi_n$ and their corresponding eigenvalues $\lambda_n$, computed from the fully observed L63 system. Top: Scatterplots of the eigenfunction values $\phi_n(x_j)$ on the covariate training data $x_j = \omega_j \in \mathbb{R}^3$. Bottom: Eigenfunction time series $t_j \mapsto \phi_n(x_j)$ over a portion of the training dataset spanning 10 natural time units. Notice that, despite the fact that the L63 attractor is not a Riemannian manifold, the eigenfunctions qualitatively resemble a generalized Fourier basis associated with a heat kernel. That is, as $\lambda_n$ decreases, $\phi_n$ exhibits increasingly small-scale oscillatory behavior, allowing one to represent functions of increasingly fine structure through eigenfunction expansions.

Figure 3: As in Figure 2 but for eigenfunctions computed from the partially observed L63 system. Top: Scatterplots of the eigenfunction values $\phi_n(x_j)$ on the L63 states $\omega_j$ underlying the covariate data $x_j \in \mathbb{R}$. Middle: Eigenfunction values $\phi_n(x_j)$ versus $x_j$. Coloring is as in the top row. Bottom: Eigenfunction time series $t_j \mapsto \phi_n(x_j)$ over a portion of the training dataset spanning 10 natural time units.
empirical standard deviation (i.e., the $L^2(p_\rho)$ norm of $Y - \int_\Omega Y \, dp_\rho$). Starting from the fully observed examples, the RMSE of all three state vector components $\omega^i$ exhibits an initial exponential-like increase from near-zero values for $\tau \lesssim 0.5 \approx 0.5/\Lambda$. This period is followed by an intermediate-time regime with more gradual RMSE increase and noticeable oscillatory behavior, until convergence to the equilibrium standard deviation (normalized RMSE $\approx 1$) at late times, $\tau \gtrsim 4$

Examining the individual forecast trajectories, it is evident that the late-time convergence of the RMSE to a near-constant values is a manifestation of the trajectories converging to the mean, $E[Y]$. The numerical results are therefore consistent with the theoretically expected late-time behavior of KAF in the presence of mixing dynamics, discussed in Section 3.3. It is also evident from Figure 4 that the error estimators $\varepsilon_{f,\ell,n}$ provide useful uncertainty quantification. That is, the error bars derived from these quantities envelope, for the most part, the true trajectories, and their RMS values agree well with the forecast RMSE.

Overall, in the fully-observed experiments, $\omega^3$ is the most predictable state vector component (likely due to symmetry of the L63 equations), followed by $\omega^1$ and $\omega^2$ which are nearly equally predictable (again due to symmetry). If one were to set a normalized RMSE value of 0.6 as a threshold for loss of skill, $\omega^3$ would remain predictable out to $\approx 3$ natural time units (i.e., $\approx 3$ Lyapunov timescales), whereas $\omega^1$ and $\omega^2$ would remain predictable out to $\tau \approx 2$. Setting that threshold to 0.8 increases the predictability horizon of $\omega^3$ and $\omega^3/\omega^2$ to $\tau \approx 5$ and 3, respectively.

Turning now to the Figure 5 results for the partially observed system, it is clear that the act of observing $\omega^1$ only in the covariate space bears a significant impact on forecast skill, particularly for $\omega^2$ and $\omega^3$. Indeed, for these state vector components, the non-injectivity of the covariate function means that the normalized RMSE can be significant even at $\tau = 0$, without ever dropping below $\lesssim 0.4$. Yet, even though the method cannot overcome the intrinsic error of this observational setup, it is nevertheless capable of providing fairly adequate uncertainty quantification, as manifested by the reasonably good ability of the estimated error bars to envelop the true trajectories (with the notable exception of certain near-extremal points) and the close agreement between the RMS values of $\varepsilon_{f,\ell,n}$ and the forecast RMSE.

As our final numerical results, we show in Figure 5 trajectory and RMSE results for prediction of the characteristic functions $\chi^i$, corresponding to the conditional probabilities for $\omega^i$ to take greater-than-average values. These forecasts were obtained using the empirical target functions $g_{f,\ell,n}$ from (23), constructed using the same parameter values as the state vector forecasts in Figure 4 based on $f_{f,\ell,n}$. Compared to forecasts of the state vector components, forecasts of characteristic functions are hampered by the fact that a characteristic function has discontinuities (apart from trivial cases), potentially inducing Gibbs oscillations in approximations by finite linear combinations of RKHS functions. Such oscillations may in turn induce overshoots outside the interval $[0, 1]$, necessitating the use of thresholding in (23). Evidence of active thresholding can be seen in Figure 5, particularly at early times ($\tau \lesssim 0.5$) where the relative RMSE is significantly larger than the corresponding state vector results in Figure 4. Despite that, the conditional probability results are broadly consistent with their state vector counterparts. That is, $\chi^1/\chi^2$ and $\chi^3$ remain predictable out to $2–3$ and $4–5$ natural time units, similarly to $\omega^1/\omega^2$ and $\omega^3$, respectively, and as expected, the fully observed forecasts fare substantially better than the partially observed ones. It is worth noting that unlike $\omega^1$, the $\chi^i$ forecasts have not converged to near-constant values at the end of the examined prediction intervals (i.e., at $\tau = 5$).

7. Conclusions

As shown throughout this paper, the theoretical underpinning of the kernel approach to forecasting is that it approximates the conditional expectation of observables, in the sense of minimizing mean square forecast error. The extent to which approximating the conditional expectation is one of the better ways of producing forecasts depends on the specific dynamical system and the goals of the forecaster, but is a natural and common target in many applications. Although there are many ways of achieving this approximation, we have shown in this article that the kernel approach is a distinguished such method both theoretically, given the central importance of Hilbert space theory for both kernels and the conditional expectation, and practically, as the computation requires only eigenfunction computation and matrix multiplication.

In contrast to the usual expositions of kernel methods that present kernels and RKHSs as an axiomatic starting point, we have followed a different order in which the appearance of kernels arises naturally within a learning framework (with hypothesis spaces as a prominent object) and with error minimization as a starting point. It is this perspective on kernel based forecasting, i.e. one that deemphasizes kernels in favor of conditional expectation, that is the main contribution of this paper.
Figure 4: Results of KAF applied to prediction of the L63 state vector components, $\omega^1$, $\omega^2$, and $\omega^3$, with covariate variables given by the full state vector (blue lines) and state vector component $\omega^1$ only (red lines). Top panels: True signal (black lines) and forecast trajectories $f_{\tau,\ell,n}$ (solid blue and red lines) as a function of lead time $\tau$, initialized from an arbitrary condition in the verification dataset. Estimated errors obtained by adding $\pm\varepsilon_{\tau,\ell,n}$ to the forecast trajectories are shown in dashed lines. Bottom panels: RMSE as a function of $\tau$ determined from the verification dataset (solid lines). Dashed lines show the RMS value of the estimated error $\varepsilon_{\tau,\ell,n}$.

Figure 5: As in Figure 4, but for prediction of the characteristic functions $\chi^1$, $\chi^2$, and $\chi^3$, representing the L63 states whose components $\omega^1$, $\omega^2$, and $\omega^3$, respectively, are greater than their mean. The initial condition in the top panels is the same as in the top panels of Figure 4.
Additionally, we presented and proved the results that the empirically obtained kernel forecasting function approaches, in the limit of large data, the ideal kernel forecasting function, which itself approaches the true conditional expectation as more principal components (kernel eigenfunctions) are utilized. Precise estimates on the rate of convergence is an active area of research and one that depends on specific aspects of both the dynamical system and the employed kernels.

One of the advantages of an understanding of kernel forecasting based on conditional expectation, so we have argued, is that it enables the computation of a host of related quantities, including conditional probability and conditional variance. The former can be used to handle the binary classification problem that arises when trying to detect extreme or rare events. The latter, meanwhile, is instrumental in providing more informative forecasts that detail the level of uncertainty involved. Another benefit of the statistical learning framework is that it shows the connection between the two most common kernel methods, KPCR (of which KAF is an example) and KRR; in particular, they both follow the same variational logic, but the former is based on a choice of a linear hypothesis space whereas the latter uses a nonlinear one. Although KRR may be a simpler algorithm to implement, and is more accurate in the presence of noise, KPCR can converge much more rapidly when the predictand happens to lie in the space spanned by the leading principal components.

Applications of KAF to two low-dimensional dynamical systems were presented for the sake of illustration. The first system, periodic flow on a circle, is in fact not a system for which conditional expectation is a good estimate of forecasts, at least when the abscissa is the only quantity on which the forecast is conditioned. Nevertheless, we demonstrate that KAF implemented with a radial Gaussian kernel converges to this conditional expectation quite rapidly, and that the dependence of its error on the number of principal components follows a U-shaped curve that is characteristic of the classic bias-variance tradeoff of statistical learning. The second system, the L63 system, exhibits a number of the hallmark challenges in forecasting of complex systems, including invariant measures supported on complicated sets (fractal attractors) and mixing dynamics. Despite these challenges, we saw that KAF, implemented with a judiciously chosen variable-bandwidth, Markov-normalized Gaussian kernel, successfully predicts the state vector components, as well as their associated conditional probabilities to take greater-than average values. As expected, conditioning on the full state produces better forecasts than conditioning on just partial observations of the state, but in both cases the method yielded adequate uncertainty quantification through estimates of the conditional variance. This example also demonstrates that forecasts based on partial conditioning are better for some choices of response variables than others (in particular, the first coordinate of the L63 has greater predictive value for the third coordinate than for the second coordinate).

There are two chief challenges in utilizing kernel methods in real-world applications. The first is an appropriate choice of response, as well as a covariate variable with sufficiently rich predictive value. The second challenge, particularly when dealing with very high-dimensional covariate spaces, is a choice of kernel such that as much of the dynamical features of interest can be characterized by as few of the leading principal components as possible. In general, the response and covariate are selected with the certainty that there is close association between the two, but with the precise nature of the correspondence being either unknown, or intractable to reproduce analytically or numerically. In real-world applications, this issue is further compounded by the fact that the response space is oftentimes multi-dimensional. While in this paper we did not directly address this situation, it is natural to consider extensions of KAF to the setting of vector-valued response functions using operator-valued kernel techniques [69] for multi-task learning. As for the choice of kernel, recent approaches for learning kernels targeted to specific response functions [71] could potentially provide effective ways of ensuring that the response is well-captured by the leading eigenspaces of the corresponding integral operator, thus improving forecast skill. The main goal of this paper has been to clarify the theoretical justification for utilizing kernels in forecasting observables of dynamical systems, so that the forecaster can focus on the remaining problem of leveraging specific scientific knowledge of the system into optimal choices of response, covariate, and kernel.

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References

[1] E. Lorenz, Atmospheric predictability as revealed by naturally occurring analogues, J. Atmos. Sci. 26 (1969) 636–646. doi:10.1175/1520-0469(1969)26<636:apa>2.0.co;2
[2] J. D. Farmer, J. J. Sidorowich, Predicting chaotic time series, Phys. Rev. Lett. 59 (8) (1987) 845–848. doi:10.1103/PhysRevLett.59.845
[3] M. Casdagli, Nonlinear prediction of chaotic time series, Physica D 35 (3) (1989) 335–356. doi:10.1016/0167-2789(89)90074-2
[4] T. Sauer, Time series prediction by using delay coordinate embedding, in: A. S. Weigend, N. A. Gerbenfeld (Eds.), Time Series Prediction: Forecasting the Future and Understanding the Past, Vol. 15 of SFI Studies in the Sciences of Complexity, Addison-Wesley, 1993, pp. 175–193.
[5] J. Fan, Q. Yao, Nonlinear time series: nonparametric and parametric methods, Springer Science & Business Media, 2008.
[6] Z. Zhao, D. Giannakis, Analog forecasting with dynamics-adapted kernels, Nonlinearity 29 (2016) 2888–2939. doi:10.1088/0951-7715/29/9/2888
[7] L. Delle Monache, T. Nipen, Y. Liu, G. Roux, R. Stull, Kalman filter and analog schemes to postprocess numerical weather predictions, Mon. Weather Rev. 139 (11) (2011) 3554–3570.
[8] A. Atencia, I. Zawadski, A comparison of two techniques for generating ensembles. Part II: Analog selection and comparison of techniques, Mon. Weather Rev. 143 (2015) 2890–2908. doi:10.1175/MWR-D-14-00342.1
[9] R. Alexander, Z. Zhao, E. Szekely, D. Giannakis, Kernel analog forecasting of tropical intraseasonal oscillations, J. Atmos. Sci. 74 (2017) 1321–1342. doi:10.1175/JAS-D-16-0147.
[10] D. Comeau, Z. Zhao, D. Giannakis, A. J. Majda, Data-driven prediction strategies for low-frequency patterns of North Pacific climate variability, Climate Dyn. 48 (5-6) (2017) 1855–1872. doi:10.1007/s00382-016-3177-5
[11] D. Comeau, D. Giannakis, Z. Zhao, A. J. Majda, Predicting regional and pan-arctic sea ice anomalies with kernel analog forecasting, Climate Dyn. 52 (9-10) (2019) 5507–5525. doi:10.1007/s00382-018-4459-x
[12] C. Voyant, M. L. Nivet, C. Paoli, M. Muselli, G. Notton, Meteorological time series forecasting based on mlp modelling using heterogeneous transfer functions, in: J. Phys. Conf. Ser., Vol. 574, IOP Publishing, 2015, p. 012064.
[13] K. Chakraborty, K. Mehrotra, C. K. Mohan, S. Ranka, Forecasting the behavior of multivariate time series using neural networks, Neurot. Netw. 5 (6) (1992) 961–970. doi:10.1016/0893-6080(92)90092-9
[14] N. K. Ahmed, A. F. Aliya, N. E. Gayar, H. El-Shishiny, An empirical comparison of machine learning models for time series forecasting, Econom. Rev. 29 (5-6) (2010) 594–621. doi:10.1016/j.estr.2015.05.001
[15] M. A. Aizerman, Theoretical foundations of the potential function method in pattern recognition learning, Autom. Remote Control 25 (1964) 821–837.
[16] B. E. Boser, I. M. Guyon, V. N. Vapnik, A training algorithm for optimal margin classifiers, in: Proceedings of the fifth annual workshop on Computational learning theory, ACM, 1992, pp. 144–152.
[17] T. Hofmann, B. Schölkopf, A. J. Smola, Kernel methods in machine learning, Ann. Stat. (2008) 1171–1220.
[18] H. Drucker, C. J. Burges, L. Kaufman, A. J. Smola, V. Vapnik, Support vector regression machines, in: Adv Neural Inf Process Syst, 1997, pp. 155–161.
[19] C. Saunders, A. Gammerman, V. Vovk, Ridge regression learning algorithm in dual variables, ICML-1998 Proceedings of the 15th International Conference on Machine Learning (04 1999).
[20] R. Rosipal, L. J. Trejo, A. Cichocki, Kernel principal component extraction, Tech. rep., University of Paisley, Scotland (2000).
[21] K.-R. Müller, A. J. Smola, G. Rätsch, B. Schölkopf, J. Kohlmorgen, V. Vapnik, Predicting time series with support vector machines, in: International Conference on Artificial Neural Networks, Springer, 1997, pp. 999–1004.
[22] P. Exterkate, P. J. Groenen, C. Heij, D. van Dijk, Nonlinear forecasting with many predictors using kernel ridge regression, Int. J. Forecast. 32 (3) (2016) 736–751. doi:10.2139/astm.1738192
[23] F. E. Tay, L. Cao, Application of support vector machines in financial time series forecasting, Omega 29 (4) (2001) 309–317. doi:10.1016/S0305-0488(01)00026-3
[24] V. N. Vapnik, An overview of statistical learning theory, IEEE Trans. Neural Netw. 10 (5) (1999) 988–999. doi:10.1109/72.788600
[25] F. Cucker, D. Zhou, Learning Theory: An Approximation Theory Viewpoint, Cambridge monographs on applied and computational mathematics, Cambridge University Press, 2007.
[26] V. Kuznetsov, M. Mohri, Learning theory and algorithms for forecasting non-stationary time series, in: Adv. Neural Inf. Process. Syst., 2015, pp. 541–549.
[27] V. Kuznetsov, M. Mohri, Time series prediction and online learning, in: Conference on Learning Theory, 2016, pp. 1190–1213.
[28] P. Collet, Dynamical systems and stochastic processes (2008). URL https://www.cimat.mx/Eventos/meas09/cursocollet.pdf
[29] T. Eisner, B. Farkas, M. Haase, R. Nagel, Operator theoretic aspects of ergodic theory, Vol. 272, Springer, 2015.
[30] M. Budisić, R. Mohr, I. Mezić, Applied Koopmanism, Chaos 22 (2012) 047510. doi:10.1063/1.4772195
[31] B. O. Koopman, Hamiltonian systems and transformation in Hilbert space, Proc. Natl. Acad. Sci. 17 (5) (1931) 315–318. doi:10.1073/pnas.17.5.315
[32] M. Korda, I. Mezić, Linear predictors for nonlinear dynamical systems: Koopman operator meets model predictive control, Automatica 93 (2018) 149–160. doi:10.1016/j.automatica.2018.03.066
[33] M. O. Williams, I. G. Kevrekidis, C. W. Rowley, A data-driven approximation of the Koopman operator: Extending dynamic mode decomposition, J. Nonlinear Sci. 25 (6) (2015) 1307–1346. doi:10.1007/s00332-015-9258-5
[34] M. Dellnitz, O. Junge, On the approximation of complicated dynamical behavior, SIAM J. Numer. Anal. 36 (1999) 491. doi:10.1137/S0036142996313002
[35] I. Mezić, Spectral properties of dynamical systems, model reduction and decompositions, Nonlinear Dyn. 41 (2005) 309–325. doi:10.1007/s11071-005-2824-x
[36] D. Giannakis, Data-driven spectral decomposition and forecasting of ergodic dynamical systems, Appl. Comput. Harmon. Anal. In press (2017). doi:10.1016/j.acha.2017.09.001
[37] J. C. Ferreira, V. A. Menegato, Positive definiteness, reproducing kernel Hilbert spaces, and beyond, Ann. Funct. Anal. 4 (2013) 64–88. doi:10.1582/aifa/1398599588
[38] E. N. Lorenz, Deterministic nonperiodic flow, J. Atmos. Sci. 20 (1963) 130–141. doi:10.1175/1520-0469(1963)020<0130:DNF>2.0.CO;2
[39] B. O. Koopman, Hamiltonian systems and transformation in Hilbert space, Proc. Natl. Acad. Sci. U.S.A. 17 (5) (1931) 315.
[40] O. Christensen, Operators with closed range, pseudo-inverses, and perturbation of frames for a subspace, Canad. Math. Bull. Vol. 42 (1) (1999) 37–45. doi:10.4153/CMB-1999-004-5
[41] R. R. Coifman, S. Lafon, Geometric harmonics: A novel tool for multiscale out-of-sample extension of empirical functions, Appl. Comput. Harmon. Anal. 21 (2006) 31–52. doi:j.acha.2005.07.006
[42] A. Aronszajn, Theory of reproducing kernels, Trans. Amer. Math. Soc. 63 (1950) 337–404. doi:10.1090/S0002-9947-1950-0051377-0
[43] C. M. Brislawn, Traceable integral kernels on countable generated measure spaces, Pacific J. Math. 150 (2) (1991) 229–240.
[44] T. Berry, D. Giannakis, J. Harlim, Nonparametric forecasting of low-dimensional dynamical systems, Phys. Rev. E. 91 (2015) 032915. doi:10.1103/PhysRevE.91.032915
[45] R. R. Coifman, S. Lafon, Diffusion maps, Appl. Comput. Harmon. Anal. 21 (2006) 3–30. doi:j.acha.2006.04.006
[46] U. von Luxburg, M. Belkin, O. Bousquet, Consistency of spectral clustering, Ann. Stat. 26 (2) (2008) 555–586. doi:10.1214/009053607000000640
[47] R. Coifman, M. Hirn, Bi-stochastic kernels via asymmetric affinity functions, Appl. Comput. Harmon. Anal. 35 (1) (2013) 177–180. doi:j.acha.2013.01.001
[48] T. Berry, J. Harlim, Variable bandwidth diffusion kernels, Appl. Comput. Harmon. Anal. 40 (1) (2016) 68–96. doi:10.1016/j.acha.2015.01.001
[49] H. Köng, Eigenvalue Distribution of Compact Operators, Vol. 16 of Operator Theory: Advances and Applications, Birkhäuser, Basel, 1986.
[50] J. C. Ferreira, V. A. Menegatto, Eigenvalues of integral operators defined by smooth positive definite kernels, Integr. Equ. Operator Theory 64 (2009) 61–81. doi:10.1007/s00020-009-1680-3
[51] J. Ferreira, V. A. Menegatto, Eigenvalue decay rates for positive integral operators, Ann. Mat. Pura Appl. 192 (6) (2013) 1025–1041. doi:10.1007/s10231-012-0256-2
[52] K. Law, A. Shukla, A. M. Stuart, Analysis of the 1DVAR filter for the partially observed Lorenz’63 model, Discrete Contin. Dyn. Syst. 3 (3) (2013) 1061–1078. doi:10.3934/dcds.2014.34.1061
[53] P. Constantin, C. Foias, B. Nicolaenko, R. Temam, Integral Manifolds and Inertial Manifolds for Dissipative Partial Differential Equations, Springer, New York, 1989. doi:10.1007/978-1-4612-3506-4
[54] L. S. Young, What are SRB measures, and which dynamical systems have them?, J. Stat. Phys. 108 (2002) 733–754. doi:10.1023/A:1010762724717
[55] S. Das, D. Giannakis, Delay-coordinate maps and the spectra of Koopman operators, J. Stat. Phys. in press (2019). doi:10.1007/s10955-019-02272-w
[56] D. Giannakis, A. Ourmazd, J. Slawinska, Z. Zhao, Spatiotemporal pattern extraction by spectral analysis of vector-valued observables, J. Nonlinear Sci., in press (2019). doi:10.1007/s00332-019-09548-1
[57] P. Walters, An Introduction to Ergodic Theory, Vol. 79 of Graduate Texts in Mathematics, Springer-Verlag, New York, 1981.
[58] C. A. Micchelli, Interpolation of scattered data: Distance matrices and conditionally positive definite functions, Constr. Approx. 2 (1986) 11–22. doi:10.1007/BF01893614
[59] M. C. Genton, Classes of kernels for machine learning: A statistics perspective, J. Mach. Learn. Res. 2 (2001) 299–312.
[60] P. Holmes, J. L. Lumley, G. Berkooz, Turbulence, Coherent Structures, Dynamical Systems and Symmetry, Cambridge University Press, Cambridge, 1996.
[61] C. Penland, Random forcing and forecasting using principal oscillation pattern analysis, Mon. Weather Rev. 117 (10) (1989) 2165–2185. doi:10.1175/1520-0493(1989)117<2165:RFAPUP>2.0.CO;2
[62] S. Das, D. Giannakis, Koopman spectra in reproducing kernel Hilbert spaces (2018). arXiv:1801.07799
[63] L. Zelnik-Manor, P. Perona, Self-tuning spectral clustering, in: Advances in Neural Information Processing Systems, Vol. 17, 2004, pp. 1601–1608.
[64] S. Das, D. Giannakis, J. Slawinska, Reproducing kernel Hilbert space compactification of unitary evolution groups (2019). arXiv:1808.03515
[65] W. Tucker, The Lorenz attractor exists, C. R. Acad. Sci. Paris, Ser. I 328 (1999) 1197–1202.
[66] M. J. McGinness, The fractal dimension of the Lorenz attractor, Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. 262 (1968) 413–458. doi:10.1098/rsta.1968.0001
[67] J. C. Sprott, Chaos and Time-Series Analysis, Oxford University Press, Oxford, 2003.
[68] S. Luzzatto, I. Melbourne, F. Paccaut, The Lorenz attractor is mixing, Comm. Math. Phys. 260 (2) (2005) 393–401. doi:10.1007/s00220-005-1411-9
[69] C. A. Micchelli, M. Pontil, On learning vector-valued functions, Neural Comput. 17 (1) (2005) 177–204. doi:10.1162/0899766057743802
[70] J. Slawinska, A. Ourmazd, D. Giannakis, A new approach to signal processing of spatiotemporal data, in: IEEE Statistical Signal Processing Workshop, Freiburg, Germany, 2018. doi:10.1109/SSP.2018.840704
[71] O. Ow haci, G. R. Yoo, Kernel flows: From learning kernels from data into the abyss, J. Comput. Phys. 389 (2019) 22–47. doi:10.1016/j.jcp.2019.03.040