A NEW APPROACH TO SIGNAL PROCESSING OF SPATIOTEMPORAL DATA

Joanna Slawinska, Abbas Ourmazd
Department of Physics
University of Wisconsin-Milwaukee
Milwaukee, WI

Dimitrios Giannakis
Courant Institute of Mathematical Sciences
New York University
New York, NY

ABSTRACT
We present a method combining ideas from the theory of operator-valued kernels with delay-coordinate embedding techniques in dynamical systems capable of identifying spatiotemporal patterns, without prior knowledge of the state space or the dynamical laws of the system generating the data. The approach is particularly powerful for systems in which characteristic patterns cannot be readily decomposed into temporal and spatial coordinates. Using simulated and observed sea-surface temperature data, we show our approach reveals coherent patterns of intermittent character with significantly higher skill than conventional analytical methods based on decomposing signals into separable spatial and temporal patterns.

Index Terms—Signal processing, kernel methods, vector-valued functions, multivariate time series, dynamical systems, spatiotemporal patterns

1. INTRODUCTION
Identifying coherent spatiotemporal patterns generated by nonlinear dynamics is a central problem in many science and engineering disciplines. Techniques for spatiotemporal pattern extraction first identify typically temporal patterns through the eigenfunctions of an operator approximated from the data, then project the data onto those eigenfunctions to obtain corresponding spatial patterns, finally combining the temporal and spatial patterns through products to obtain spatiotemporal modes. For example, spatiotemporal pattern extraction through principal components analysis (PCA) [1], diffusion maps [2], or dynamic mode decomposition [3, 4] is based on eigenfunctions of empirical covariance, heat, and Koopman operators, respectively. A common feature of these approaches is that they yield characteristic modes with a separable temporal and spatial structure. However, many signals generated by complex systems exhibit intermittency and other characteristics which render them manifestly non-separable.

In addition, many systems of interest exhibit spatial symmetries, which are also poorly represented by conventional approaches [5].

Here, we describe a new approach, called vector-valued spectral analysis (VSA) which addresses these shortcomings by taking advantage of the intrinsic structure of spatiotemporal signals as vector-valued observables of a dynamical systems. From this perspective, we employ the theory of operator-valued kernels for multitask machine learning [6] and delay-coordinate maps of dynamical systems [7] to construct kernel integral operators for data analysis that take into account both temporal and spatial dependencies. We show that this approach is able to efficiently recover non-separable spatiotemporal patterns, while also factoring out any underlying data symmetries.

2. VECTOR-VALUED SPECTRAL ANALYSIS
Consider a continuous-time dynamical system on a manifold \( X \), whose flow map \( \Phi^t : X \mapsto X, t \in \mathbb{R} \), possesses a compact invariant set \( A \subseteq X \) and an ergodic invariant probability measure \( \mu \) supported on \( A \). For instance, \( X \) could be the state space of a finite-dimensional ordinary differential equation model, or an inertial manifold of an infinite-dimensional partial differential equation (PDE) model. Let also \( Y \) be a spatial domain (which we assume to have the structure of a compact metric space), equipped with a finite measure \( \nu \), and let \( H_Y = \{ f : Y \mapsto \mathbb{C}, \int_Y |f|^2 \ d\nu < \infty \} \) be the Hilbert space of square-integrable complex-valued functions on \( Y \) associated with \( \nu \). For our purposes, \( H_Y \) will be the space of physically admissible spatial patterns generated by the dynamical system. In particular, we are interested in a scenario where there is a continuous observation function \( F : X \mapsto H_Y \) mapping each dynamical state \( x \in X \) to a spatial pattern \( F(x) \in H_Y \). Note that in PDE systems it is often the case that \( X \) is a subset of \( H_Y \); that is, states of the system are scalar fields on \( Y \), and \( F \) reduces to an inclusion map.

In general, we view \( F \) as a vector-valued observable of the dynamical system as it takes values in a vector space (in this case, a Hilbert space) of functions \( H_Y \). In particular, \( F \) lies in the Hilbert space \( \mathcal{H} = \{ f : X \mapsto \mathbb{C} \} \).
improvements to the physical interpretability of the recovered modes by incorporating tools such as delay-coordinate embeddings [7] and kernels for manifold learning [2, 11], while also providing rigorous spectral convergence guarantees on non-smooth attractors [12]. Nevertheless, these methods also impose a separable or near-separable structure in the recovered spatiotemporal patterns and suffer from similar issues as PCA in the presence of symmetries.

Arguably, the shortcomings described above can be attributed to the fact that the spatial and temporal degrees of freedom are treated separately through operators acting on scalar function spaces such as $H_X$ and $H_Y$. In that regard, our approach departs significantly from the conventional paradigm, as it is based on operators acting on the natural space $\mathcal{H}$ of vector-valued observables from the outset, without imposing restrictive separability constraints. To construct this class of operators, we take advantage of the fact that, in addition to being isomorphic to $H_X \otimes H_Y$, $\mathcal{H}$ is also isomorphic to the Hilbert space $H\mathcal{O} = \{f: \mathcal{O} \rightarrow \mathbb{C}, \int_\mathcal{O} |f|^2 \, d\mu < \infty\}$ of scalar-valued functions on the product space $\mathcal{O} = X \times Y$, square-integrable with respect to the product measure $\rho = \mu \otimes \nu$. This means that we can first construct an appropriate integral operator on $H\mathcal{O}$ based on a scalar-valued kernel on $\mathcal{O}$, and then map that operator to an equivalent operator on $\mathcal{H}$, which will be associated with an induced \textit{operator-valued kernel} [6].

Expanding on ideas introduced in NLSA, we consider a class of kernels $k_Q: \mathcal{O} \times \mathcal{O} \rightarrow \mathbb{R}$, which assign the following bounded measure of similarity $k_Q(\omega, \omega') = h(d_Q(\omega, \omega'))$ to each pair of points $(\omega, \omega') \in \mathcal{O} \times \mathcal{O}$, with $\omega = (x, y)$, $\omega' = (x', y')$, and $d_Q: \mathcal{O} \times \mathcal{O} \rightarrow \mathbb{R}$ a pseudometric on $\mathcal{O}$, parameterized by a positive integer parameter $Q$ (the number of delays), and defined by

$$d_Q^2(\omega, \omega') = \frac{1}{Q} \sum_{q=0}^{Q-1} |F((\Phi^{-q\tau}(x), y)) - F((\Phi^{-q\tau}(x'), y'))|^2.$$

Here, $h: \mathbb{R} \rightarrow \mathbb{R}$ is a bounded continuous kernel shape function, chosen so that $k_Q$ is bounded from below on compact sets. We nominally utilize a Gaussian shape function, $h(s) = e^{-s^2/\epsilon}$, parameterized by a bandwidth parameter $\epsilon > 0$, which is a standard choice in machine learning due to its connections with heat kernels on manifolds [2, 11]. In effect, $k_Q(\omega, \omega')$ is based on an averaged squared distance between $Q$-element temporal sequences of the values of the observation map $F$ at the spatial points $y, y' \in Y$ and initialized at the dynamical states $x, x' \in X$, respectively. Note that $k_Q$ is generally not expressible as a product of kernels on $X$ and $Y$.

Associated with $k_Q$ is an integral operator $K_Q: \mathcal{H} \rightarrow \mathcal{H}$ that maps $f \in H\mathcal{O}$ to $K_Q f = \int_\mathcal{O} k_Q(\cdot, \omega) f(\omega) \, d\rho(\omega)$.

Equivalently, there is a kernel integral operator $K_Q: \mathcal{H} \rightarrow \mathcal{H}$ that acts on vector-valued observables in $\mathcal{H}$ through an \textit{operator-valued kernel} $\ell_Q: X \times X \rightarrow \mathcal{L}(H_Y)$ that maps every pair $(x, x')$ of dynamical states in $X \times X$ to a bounded lin-
Fig. 1. Fundamental component of ENSO (a, d) and combination modes capturing ENSO’s interaction with the annual cycle (b, c, e, f), as derived from Indo-Pacific sea-surface temperature (SST) data by VSA (a–c) and NLSA (d–f). The VSA patterns in (a–c) are raw vector-valued eigenfunctions $\phi_j \in \mathcal{H}$, normalized to unit norm. The NLSA patterns in (d–f) are spatiotemporal SST anomaly patterns (in K), obtained from scalar-valued kernel eigenfunctions as described in [10]. All patterns are shown as functions of time $t$ and latitude $\lambda$ over a 20-year portion of the 1300-year dataset.

The operator $B = l_Q(x, x')$ acting on functions in $H_Y$ through the formula $Bg = \int_Y k_Q(x, x', y') g(y') \, d\nu(y')$, $g \in H_Y$. This leads to the action of $K_Q$ on a vector-valued observable $f \in \mathcal{H}$ given by $K_Q f = \int_X l_Q(\cdot, x) f(x) \, d\mu(x)$, where the integral in this equation is a Bochner integral. The operator $K_Q$ can be normalized to an ergodic, compact Markov operator $P_Q : H_\Omega \rightarrow H_\Omega$ with real eigenvalues, by applying the kernel normalization procedure introduced in the diffusion maps algorithm [2]. This induces a corresponding normalized operator $P_Q : \mathcal{H} \rightarrow \mathcal{H}$ acting on vector-valued observables, which is used to identify vector-valued patterns through its eigenfunctions $\phi_k \in \mathcal{H}$. The latter are used in the VSA decompositions of the input signal in (1), with the expansion coefficients $c_k = \langle \phi_k, F \rangle_H$ determined through the eigenfunctions $\phi_k$ of the adjoint of $P_Q$, satisfying $\langle \phi'_j, \phi_k \rangle_H = \delta_{jk}$. Note that both $\phi_k$ and $\phi'_k$ have scalar-valued representations in $H_\Omega$ (due to the isomorphism $\mathcal{H} \approx H_\Omega$), and the latter can be determined through the eigenfunctions of a self-adjoint operator by standard techniques [2].

A key aspect of the VSA decomposition is that the individual terms $\phi_k$ are not constrained to be products of functions on $H_X$ and $H_Y$; in fact, when dealing with complex spatiotemporal patterns, the $\phi_k$ will in general be manifestly non-separable. By convention, we order the eigenfunctions in order of decreasing eigenvalue $\lambda_j$ of $P_Q$. This has an interpretation as ordering the $\phi_k$ in increasing order of a kernel-dependent measure of “roughness” (Dirichlet energy) of functions on $\Omega$ [13, 14, 12]. In particular, by ergodicity and Markovianity of $P_Q$, the eigenvalues satisfy $1 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots$, and $\phi_0$ corresponds to a constant function on $\Omega$ which has minimal roughness. In a data-driven environment, functions with low roughness have high robustness against noise and sampling errors. Thus, the truncated expansion $F_l = \sum_{k=0}^l c_k \phi_k$ extracts from $F$ the vector-valued patterns $c_k \phi_k$ lying in the $l$-dimensional subspace of the range of $P_Q$ corresponding to maximal regularity and minimal risk of overfitting.

In addition to optimizing for regularity, the VSA decomposition is likely to yield patterns of high physical interpretability owing to the particular properties of the kernel employed. Specifically, it can be shown [8] that: (1) If the system has nontrivial symmetries associated with the action of a group on $\Omega$, then the $\phi_k$ (viewed as scalar-valued functions on $\Omega$) are constant on the orbits of an associated group action on $\Omega$ commuting with the dynamical flow map; as a result, our method can be interpreted as factoring out the natural symmetries (i.e., the symmetries commuting with the dynamics), in the data. (2) When $Q$ is small, the $\phi_k$ are approximately constant on the level sets of the observation map $F$ (viewed as a scalar function on $\Omega$); this is useful for applications requiring estimation of level sets of functions from noisy data, such as topological data analysis. (3) In the limit $Q \rightarrow \infty$, $\mathcal{P}_\infty$ commutes with the Koopman operator $U^t$ of the system governing the evolution of vector-valued observables in $\mathcal{H}$. As a result, these operators have common finite-dimensional eigenspaces (by compactness of $\mathcal{P}_\infty$), and these eigenspaces are spanned by observables with a coherent spatiotemporal evolution at intrinsic timescales of the dynamical system by virtue of the properties of Koopman eigenfunctions. (4) Data-driven approximations of these patterns obtained from the time-ordered snapshots $h_0, \ldots, h_{N-1}$ converge in an appropriate limit of large data, $N \rightarrow \infty$, even if the invariant set $A$ is non-smooth and the sampled states $x_n$ do not lie exactly on $A$. 
3. ANALYSIS OF TROPICAL PACIFIC SST DATA

Spatiotemporal pattern formation is a ubiquitous in nature, and we expect the VSA framework to be applicable in several disciplines [15, 16, 17]. Here, we demonstrate its efficacy in extracting spatiotemporal modes from sea surface temperature (SST) of the Indo-Pacific Ocean, as simulated by a comprehensive climate model (CCSM4; [18]) and observationally reconstructed in a reanalysis product (NOAA 20th Century Reanalysis [19]). The Indo-Pacific Ocean is the domain of activity of several important modes of climate dynamics on subseasonal to decadal timescales, including the El Niño Southern Oscillation (ENSO) on interannual (4–8 yr) timescales. Decades of intense research has revealed the difficulties faced by classical signal processing methods in fully encapsulating the dynamical origins of this variability; particularly ENSO’s interactions with other temporal scales [20] and the mechanisms underlying its spatial diversity and broad frequency spectrum [21]. One of the current open problems in ENSO research is to objectively characterizing the different “flavors” of ENSO, which broadly consist of typical Eastern Pacific (EP) events and more infrequent events peaking in the Central Pacific (CP).

Figure 1 shows spatiotemporal patterns corresponding to representative VSA eigenfunctions recovered from simulated SST in a CCSM4 control integration spanning 1300 yr. The data were sampled on 114 spatial gridpoints along the equator for the Pacific Ocean longitudes 140°–280°. The delay embedding window was \( Q = 48 \) (4 years). These patterns include the annual cycle (not shown here) and the fundamental component of ENSO (Fig. 1(a)), featuring basin-wide oscillations on interannual timescales along with event-by-event fluctuations of the temporal duration and spatial location of its amplitude peak (ENSO diversity). In addition, VSA recovers modes representing the interaction of ENSO and the annual cycle (Fig. 1(b, c)), which have recently received significant attention in the climate science community as they are thought to underpin ENSO’s seasonal phase locking [20, 22, 23], with potential implications for predictability. In particular, it can be verified through Fourier spectral analysis at representative spatial locations that the annual pattern and the one in Figs. 1(a) vary predominantly at the annual cycle and ENSO frequencies, \( \nu_A = 1 \text{ yr}^{-1} \) and \( \nu_{\text{ENSO}} = 0.25 \text{ yr}^{-1} \), while those in Figs. 1(b) and 1(c) vary at the combination frequencies \( \nu_A - \nu_{\text{ENSO}} \) and \( \nu_A + \nu_{\text{ENSO}} \), respectively. Each of the patterns in Fig. 1 is one of the two members of a doubly-degenerate oscillatory (90° out of phase) pair. Other leading VSA patterns (not shown here) include higher harmonics of the annual cycle and low-frequency (decadal) modes. Overall, these results demonstrate that VSA is able to recover dynamically significant patterns from the highly nonlinear multiscale dynamics taking place in this domain.

Figure 1 also shows spatiotemporal SST reconstructions obtained by NLSA [10]; a scalar-valued kernel algorithm utilizing delay-coordinate embeddings as VSA, and having an analogous commutation property with Koopman operators [14, 12], endowing the method with strong timescale separation capabilities. While NLSA also yields high-quality representations of the annual cycle, ENSO, and the associated combination modes [22, 23] (significantly improving over PCA which fails to identify these patterns as distinct modes), these representations have a low-rank, near-separable structure in the temporal and spatial coordinates. This is manifested by the NLSA ENSO pattern in Fig. 1(d), which exhibits significantly weaker event-to-event variations (ENSO diversity) than the corresponding VSA eigenfunction in Fig. 1(a).

To further demonstrate the capability of VSA to capture ENSO diversity, and assess its performance compared to NLSA, in Fig. 2 we show reconstructed SST patterns based on VSA and NLSA eigenfunctions recovered from 20th Century Reanalysis SST data (using the same spatial domain and delay embedding window as in the CCSM4 analysis). The interval shown in Fig. 2 contains a number of well-documented El Niño events, of both EP and CP type. It can readily be seen that VSA recovers both event types through a single pair of eigenfunctions, while also providing a realistic representation of event-by-event diversity. In contrast, the NLSA reconstructions have poor skill in recovering CP events, and instead capture the portion of ENSO variability associated with the more regular EP events. While CP ENSO variability should have a representation in the NLSA spectrum, this variability is spread over multiple eigenfunctions.
4. REFERENCES


