Spectral Properties of Dynamical Systems, Model Reduction and Decompositions

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Abstract

In this paper we discuss two issues related to model reduction of deterministic or stochastic processes. The first is the relationship of the spectral properties of the dynamics on the attractor of the original, high-dimensional dynamical system with the properties and possibilities for model reduction. We review some elements of the spectral theory of dynamical systems. We apply this theory to obtain a decomposition of the process that utilizes spectral properties of the linear Koopman operator associated with the asymptotic dynamics on the attractor. This allows us to extract the *almost periodic* part of the evolving process. The remainder of the process has continuous spectrum. The second topic we discuss is that of model validation, where the original, possibly high-dimensional dynamics and the dynamics of the reduced model - that can be deterministic or stochastic - are compared in some norm. Using the "statistical Takens theorem" proven in [17] we argue that comparison of average energy contained in the finite-dimensional projection is one in the hierarchy of functionals of the field that need to be checked in order to assess the accuracy of the projection.

Contents

1 Introduction

Since we now understand that - barring a "blinding new technology" - the power of computers that will be available in the foreseeable future will not allow us to compute the details of physical interactions in many of the current problems in biological and physical sciences, such as molecular conformation or turbulence, the problem of *model reduction* has percolated to the top of the pile of open problems in Applied Mathematics. The number of different approaches in this direction is large, with some of the work relying on decompositions commonly used in probability theory - such as the Proper Orthogonal Decomposition (POD) (or Karhunen-Loeve, or Singular Value Decomposition) [14], and other projection methods such as the Mori-Zwanzig formalism and optimal prediction [8], the formalism that involves replacing higher-order nonlinear terms with stochastic processes [15], scale-separation and averaging methods, balanced truncation methods developed for linear control systems, operator-theoretic projection methods and coarse time-stepping methods. A good summary of a number of these is provided by Givon et al. [12].

In these approaches an analysis of how the dynamics on the attractor of the system that is being reduced affects the reduction is seldom found although attempts have been made [5]. An exception is the approach in [1] that uses directly the asymptotic dynamics on the attractor for projection and methods of Dellnitz and collaborators (see e.g. [10]) that utilizes properties of the Perron-Frobenius operator to reduce dynamics to a Markov chain. The formalism in this paper (based on our previous work in [17]) is based on the adjoint of the Perron-Frobenius operator, the so-called Koopman operator.

In this paper we discuss two issues important for model reduction that are directly related to the asymptotic properties of the dynamics. The first is the relationship of the spectral properties of the dynamics on the attractor of the original, high-dimensional dynamical system with the properties and possibilities for model reduction. We review some specifics of the spectral theory of dynamical systems - in the form developed in [17] - in section 2. We apply this theory to obtain a new type of the decomposition, that combines spectral and POD decomposition in section 3. The second topic we discuss - in section 4 - is that of model validation, where the original, possibly high-dimensional dynamics and the dynamics of the reduced model - that can be deterministic or stochastic - are compared in some norm. In the Appendix we review the notion of phase-space partitions.

2 Spectral theory of dynamical systems

2.1 Preliminaries

We consider a dynamical system in discrete time defined by

$$x_{i+1} = T(x_i), \tag{1}$$

where $i \in \mathbb{Z}$, $x_i \in M$, a compact Riemannian manifold endowed with the Borel sigma algebra and a measure ν. We assume that $T : M \to M$ is measurable map. Let f be a real or complex function on M. We call the function f^* the time average of a function f under T if

$$f^*(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} f(T^i x),$$

almost everywhere (a.e.) with respect to the measure ν on M. The time average f^* is a function of the initial state x. A good reference for the foregoing definitions is [16]. Note that by Birkhoff's pointwise ergodic theorem [19], if T is measure-preserving, f^* exists for every function $f \in L^2_\nu(M)$ (in fact this is true for any $f \in L^1_\nu(M)$, but we are going to need Hilbert space properties later). The whole formalism that we develop is valid for $\mathcal{B}$-regular systems [17]: those for which f^* exists for every continuous f. This clearly includes systems that preserve a smooth invariant measure such as Hamiltonian systems, but also includes systems that possess a physical measure [31]. A physical measure of the system $T : M \to M$ is a measure μ on M such that, for every continuous $\phi : M \to \mathbb{R}$, for almost every $m \in M$ with respect to ν (the original measure on M!)

$$\lim_{n\to\infty} \frac{1}{n} \sum_{j-0}^{n-1} \phi(T^j(m)) = \int_M \phi(m) d\mu(m).$$

Note that this can also stand as the definition of ergodicity of the measure μ if we replace the condition "for almost every $m \in M$ with respect to ν" with "for almost every $m \in M$ with respect to μ". In the case when M is a positive Lebesgue measure subset of $\mathbb{R}^n$, ν is typically chosen to be the restriction of the Lebesgue measure to that subset. In the case when M is a smooth manifold endowed with a volume form, ν is usually taken to be the volume of a set. From this point on we assume that μ is an invariant measure of a $\mathcal{B}$-regular system. The consideration of the original measure ν on M is done here only to insure that the results are valid for almost every initial condition we are interested in (and thus with respect to an a-priori measure ν).

2.2 Spectral decomposition of the Koopman operator

We now introduce the Koopman operator $U : L^2_\mu \to L^2_\mu$ (and from this point on we drop the dependence of the function space on μ from the notation), which is defined by

$$Uf(x) = f \circ T(x),$$

Note that f^* is an eigenfunction corresponding to eigenvalue 1 of the Koopman operator as f^* is constant on orbits i.e. $Uf^*(x) = f^*(x)$. Since U is unitary [19], its spectrum is restricted to the unit circle in the complex plane. U admits a unique decomposition into its singular and regular parts [20],

$$U = U_s + U_r,$$

where U_s is defined on $H_1 \subset L^2(M)$ and U_r on its orthogonal complement, H_2. Moreover, U_s has a pure discrete spectrum, determined by the eigenvalues of U, and U_r has a continuous spectrum. In fact,

$$U_s = \sum_i \lambda_i P_{\lambda_i}, \tag{2}$$

where λ_i are eigenvalues, and P_{λ_i} the projection operators to the eigenspace associated with the eigenvalue λ_i. Also,

$$U_r = \int_{S^1} e^{i2\pi\theta} dE(\theta), \tag{3}$$

where the spectral measure $dE(\theta)$ is continuous.

2.3 Invariant partitions and eigenfunctions of the Koopman operator

Throughout the paper we will assume that T is ergodic with respect to μ since that restriction is easily removed by considering the notion of the ergodic partition [16, 18]. It is important to notice that notion of ergodicity here is meant in the sense of existence of a physical measure (see (2.1) and the comment after that equation) and thus in particular systems that are dissipative with respect to ν can be ergodic with respect to μ (Example: $x' = -\lambda x$ with $|\lambda| < 1$, defined on the interval $I = [0, 1]$, where ν is the Lebesgue measure on I and ν is the Dirac delta measure at 0).

Since T is ergodic with respect to μ, every eigenvalue of U is simple [26]. The operator $P_T : L^2 \to L^2$ such that $P_T(f) = f^*$ is called the time-averaging operator. It can be considered as a member of a family of operators P^ω_T,

$$[P^\omega_T(f)](x) = f^*_\omega(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} e^{i2\pi j\omega} f(T^j(x)),$$

where $\omega \in [-0.5, 0.5)$. Note that $P_T = P^0_T$. Note that $f(T^j(x))$ is the time series of the observable f on the trajectory of the system T starting at the point

x at time 0. Thus, for fixed x, $f^*_\omega(x)$ is just the Fourier transform of this time series, and it is simple to calculate using FFT.

Like the time-averages, the functions f^*_ω also play an important role in the spectral analysis of U: they are the eigenfunctions associated with eigenvalues $e^{-i2\pi\omega}$ [19]:

$$
\begin{aligned}
Uf^*_\omega(x) &= \lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1} e^{i2\pi j\omega} f(T^{j+1}(x)) \\
&= e^{-i2\pi\omega}\lim_{n\to\infty}\frac{1}{n}\sum_{j=0}^{n-1} e^{i2\pi(j+1)\omega} f(T^{j+1}(x)) = e^{-i2\pi\omega} f^*_\omega(x).
\end{aligned}
$$

Eigenfunctions of U (and thus of U_s) can only be of the form f^*_ω: in fact a nonzero P^ω_T is the orthogonal projection operator onto the eigenspace of U associated with the eigenvalue $e^{-i2\pi\omega}$ (see the first remark on pg. 215 in [30]). It is easy to deduce using methods in [29] that existence of these averages is true for all $\mathcal{B}$-regular T's, as the existence of harmonic averages depends only on the existence of certain autocorrelations which in turn depends on the existence of time-averages of functions. P^ω_T is nonzero only on at most a countable set of ω's (Lemma in section 4 of [29]). But, when it is non-zero, it can provide substantial new information about the process that we are studying. As an application we consider how eigenfunctions of U are related to invariant partitions of the system. Clearly, the level sets of eigenfunctions at eigenvalue 1 - the time averages - produce partition of the phase space into invariant sets [18]. Consider an eigenfunction of U, f^*_ω associated with the eigenvalue $e^{-i2\pi\omega}$ with $\omega \neq 0$. Consider the partition $\zeta_{f^*_\omega}$ of the phase space into the level sets of f^*_ω, consisting of sets $B_c = (f^*_\omega)^{-1}(c), c \in S^1$. Then $T^{-1}(B_c) = B_{e^{i2\pi\omega}c}$, i.e. the dynamical system leaves the partition $\zeta_{f^*_\omega}$ invariant[1].

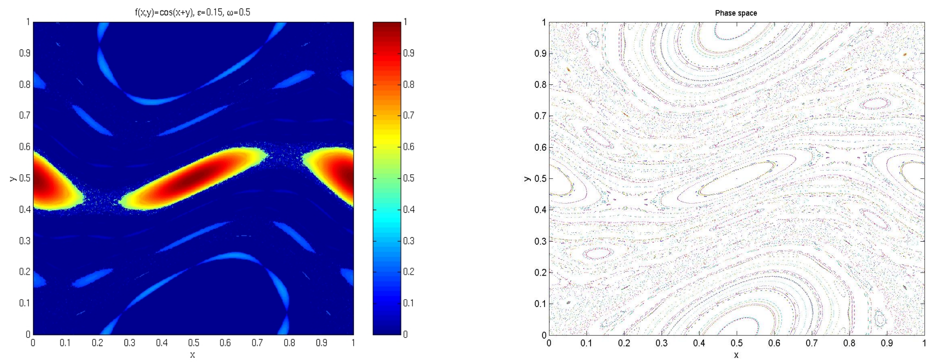
Before we go on to describe an example, we note that the case of $P^0_T = P_T$ the theory of invariant measures provides a connection of objects defined on the phase space M with the properties of P_T. Such a connection for P^ω_T was developed in [17] by showing that it is associated with certain complex measures on M.

Consider the standard map on a torus, given by

$$
\begin{aligned}
I' &= I + \epsilon\sin(2\pi\theta), \qquad \mod 1 \\
\theta' &= \theta + I + \epsilon\sin(2\pi\theta), \qquad \mod 1
\end{aligned} \tag{4}
$$

Physically, this can be derived as a Poincaré map of a plane pendulum kicked periodically with an impulsive force. In the figure 1a we show contour plot visualizing the level sets of the finite harmonic average of the function $\cos(x+y)$ for $\omega = 1/2$. In the figure 1b we show the trajectories of the map for the same

[1] For the definition of an invariant partition, and of a periodic partition, see the Appendix.



(a) (b)

Figure 1: a) Contour plot showing the level sets of $\cos(x+y)^*_{1/2}$. The parameter $\epsilon = 0.15$. b) Phase space plot of the standard map for 10000 initial conditions on a regular 100×100 grid. The parameter $\epsilon = 0.15$.

parameter value, $\epsilon = 0.15$. It is clear that the harmonic average selects the chain of sets of period 2. What is meant by this is that the level sets are sets in an invariant partition, with the system "jumping" between different sets in this partition. The system comes back to the set in the partition it started from in the second iterate. A partition with this property is called "periodic" (see the Appendix).

2.4 Random dynamical systems

Now we consider spectral theory for random dynamical systems [3]. We will work with the Discrete Random Dynamical System (DRDS) defined by

$$\begin{aligned} x_{i+1} &= T(x_i, \xi_i), \\ \xi_{i+1} &= S(\xi_i), \qquad (5) \\ & \qquad (6) \end{aligned}$$

where $i \in \mathbb{Z}, x \in M$ a compact Riemannian manifold, $\xi = \{..., \xi^{-1}, \xi^0, \xi^1, ...\} \in N^{\mathbb{Z}}$, i.e. $\xi^j \in N$, where N is a compact Riemannian manifold endowed with a probability measure p that is absolutely continuous with respect to the Lebesgue measure on N. The product space $N^{\mathbb{Z}}$ is endowed with the standard product measure Ω. S is the shift transformation $S\{..., \xi^{-1}, \xi^0, \xi^1, ...\} = \{..., \xi^0, \xi^1, \xi^2, ...\}$. We consider observables $f : M \to \mathbb{R}$ or $\mathbb{C}, f \in L^1(M)$. We denote $T^i_\xi(x) = T_{\xi^{i-1}} \circ ... \circ T_{\xi^0}$ where $T_{\xi^j}(x) = T(x, \xi^j)$. We assume that $T_\xi(x)$ is $C^r, r \geq 1$ in

x for every $\xi \in N$. With some abuse of notation, we will call the above DRDS T (note that T denotes a family of transformations indexed over ξ, rather than any particular superposition). A probabilistic measure μ on M endowed with the Borel sigma algebra is invariant for measurable T iff

$$\mathbb{E}[\mu(T^{-1}(B,\xi))] = \mu(B)$$

for every measurable B where $\mathbb{E}[\mu(T^{-1}(B,\xi))] = \int_{N^{\mathbb{Z}}} \mu(T^{-1}(B,\xi))d\Omega(\xi)$. The analogue of the Koopman operator is the *stochastic Koopman operator* U_s defined by

$$U_s f(x) = \mathbb{E}[f \circ T(x,\xi)],$$

where $\mathbb{E}[f \circ T(x,\xi)] = \int_{N^{\mathbb{Z}}} f \circ T(x,\xi)d\Omega(\xi)$. The *expectation of the time-average of* f under T is given by

$$\mathbb{E}f^*(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} U_s^i f(x). \tag{7}$$

The partition of M into level sets of $\mathbb{E}f^*$ is denoted by ζ_f. An ergodic measure on M is an invariant measure μ such that $\mathbb{E}f^*(x) = \int_M f(x)d\mu(x)$ a.e. on M for every $f \in L^1(M)$.

The family of operators $\mathbb{E}P_T^\omega$,

$$\mathbb{E}P_T^\omega(f) \equiv \mathbb{E}f_\omega^* = \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} e^{i2\pi j\omega} U_s^i f,$$

plays the role analogous to the family P_T^ω in the deterministic case. In particular, a nonzero $\mathbb{E}P_T^\omega$ is the orthogonal projection operator onto the eigenspace of U_s associated with the eigenvalue $e^{-i2\pi\omega}$.

Example 1 *Consider a map T on the interval $I = [-1,1]$ such that $T = -(2x)$* mod $[-1,1]$ *(see figure 2). At every step, every point in $[0,1]$ is mapped into $[-1,0]$ and vice versa. If we could only measure the observable* $\mathrm{Re}(F) : I \to \mathbb{R}$ *which is defined by*

$$F(x) = 1, \ \textit{for} \ \ x \in [0,1) \tag{8}$$

$$F(x) = -1, \ \textit{for} \ \ x \in [-1,0] \tag{9}$$

the behavior we would measure would be pure cycling from -1 to 1. Note that F is clearly an eigenfunction of the Koopman operator U at $\omega = 1/2$, since $F(Tx) = e^{-i\pi}F(x) = -1 \cdot F(x)$.

Now consider the random dynamical system

$$T_\xi : x' = [x] + \xi,$$

where

$$[x] = -0.5, \ \textit{for} \ \ x \in [0,1) \tag{10}$$

$$[x] = 0.5, \ \textit{for} \ \ x \in [-1,0] \tag{11}$$

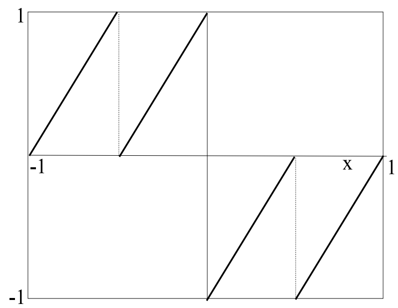


Figure 2: The map considered in Example 1

and ξ is a random variable uniformly distributed on $[0,1]$*. We have*

$$U_s F(x) = \mathbb{E}[F \circ T(x,\xi)] = e^{-i\pi} F(x),$$

and thus $F(x)$ is an eigenfunction for U_s at eigenvalue $\lambda = -1$. There are no other eigenvalues for either U or U_s. Thus, the Koopman operator of the random dynamical system T_ξ has the same point spectrum as the Koopman operator of T.

3 Spectral decomposition for evolution equations

3.1 Evolution equations and Koopman operator

Consider a discrete-time evolution equation on an infinitely-dimensional Hilbert space $\mathcal{H}$ of square-integrable vector functions on a set A given by

$$v^{n+1}(x) = N(v^n(x), p), \tag{12}$$

where $v^i : A \to \mathbb{R}^l, l \geq 1, x \in A, i \in \mathbb{Z}, N : \mathcal{H} \to \mathcal{H}$ a nonlinear operator and $p \in P$, a parameter space. To keep an example in mind, N could be a time-discretization of the flow (meant in dynamical systems sense, not fluid mechanical sense here) induced by incompressible Navier-Stokes equations defined on a 2-dimensional bounded domain A in which case $\mathcal{H}$ is the space of square-integrable volume-preserving vector fields on A. For equations arising from mathematical physics (and in particular for the aforementioned incompressible Navier-Stokes equations) it is often the case that the attractor dimension is bounded so that the essential dynamics is finite-dimensional [27]. Let us denote the attractor by M, and let m denote a point on the attractor. The dynamics of (12) restricted to M will be denoted by

$$m^{n+1} = T(m^n, p), \tag{13}$$

The original evolution variable v can be considered a vector-valued function of the phase space point m and x, $v(x,m)$. Thus $v(x,\cdot) \equiv v_x$ represents a family of observables on M parametrized by x. Note that

$$v^n(x, v^0) = v(x, m^n), \tag{14}$$

where $v^0 = v(x, m^0)$.

Example 2 *Consider the discrete nonlinear wave equation*

$$v^{n+1}(x) = F^1(v^n(x+p)),$$

where $x \in S^1$, v is a real, zero-mean periodic function in $L^2\left(S^1\right)$, F is a Fourier-space defined operator, such that if

$$f(x) = \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty} a_j \exp(i2\pi jx),$$

then

$$F^1 f(x) = \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty} \frac{\lambda a_j(|a_j|-1)}{j^2} \exp(i2\pi jx),$$

where $0 < \lambda < 1$. It is then easy to see that the attractor consists of a set of functions defined in Fourier space by $|a_1| = |a_{-1}| = 1$. Since v is real we have $\bar{a}_1 = a_{-1}$. Thus the attractor is a circle. Any point on the attractor is of the form

$$\begin{aligned}
g(x) &= a_1 \exp(i2\pi x) + a_{-1}\exp(-i2\pi x) \\
&= \exp(i2\pi\theta_1)\exp(i2\pi x) + \exp(i2\pi\theta_{-1})\exp(-i2\pi x) \\
&= \exp(i2\pi\theta_1)\exp(i2\pi x) + \exp(-i2\pi\theta_1)\exp(-i2\pi x) \\
&= v(x, \theta_1)
\end{aligned}$$

(due to $\bar{a}_1 = a_1, \theta_{-1} = -\theta_1$). The first iterate of g reads

$$\begin{aligned}
g'(x) &= a_1\exp(i2\pi(x+p)) + a_{-1}\exp(-i2\pi(x+p)) \\
&= \exp(i2\pi(\theta_1+p))\exp(i2\pi x) + \exp(-i2\pi(\theta_1 - +p))\exp(-i2\pi x),
\end{aligned}$$

and the dynamics on the attractor is given by

$$m^{n+1} = T(m,p) = m^n + p,$$

(cf. equation (13)). Also, taking the initial condition on the attractor to be θ_1, the n-th iterate of g becomes

$$g^n(x) = \exp(i2\pi(\theta_1+np))\exp(i2\pi x)+\exp(-i2\pi(\theta_1+np))\exp(-i2\pi x) = v(x, m^n),$$

(cf. equation (14)). If p is irrational, the Haar measure on S^1 is an invariant ergodic measure for T.

Consider now the finite-dimensional dynamical system (13). We assume that there is an ergodic invariant measure on the attractor M, denoted by μ. The observables v_x are continuous on the compact space M, and thus $v_x \in L^2(M)$. As discussed in the previous section, the dynamical system T induces a linear unitary operator U on M. Note that

$$U^n v_x(m^0) = v_x \circ T^n(m^0) = v_x(m^n) = v^n(x, v^0),$$

thus linking the evolution equation (12) and iteration of the Koopman operator U.

3.2 Almost periodic mean of the process

We note that if f is an eigenfunction of U with eigenvalue λ, then so is $\bar{f}$, with eigenvalue $\bar{\lambda}$. If f_1, f_2 are unit norm eigenfunctions of U associated with eigenvalues $e^{i2\pi\omega_1}, e^{i2\pi\omega_2}, \omega_1 \neq \omega_2$, then they are orthonormal since

$$\int_M f_1 \bar{f}_2 d\mu = \int_M U f_1 U \bar{f}_2 d\mu = e^{i2\pi(\omega_1-\omega_2)} \int_M f_1 \bar{f}_2 d\mu,$$

where $\bar{f}_2$ is the complex-conjugate of f_2. Thus, $\int_M f_1 \bar{f}_2 d\mu = 0$. Let $\{f_j\}, j = 1, ..., k$ (where k is possibly infinity) be an orthonormal set of eigenfunctions of U, spanning H_1 and $\exp(i2\pi\omega_j) = \lambda_j$ the associated eigenvalues. Recalling 2 and 3, for a continuous $g(x, m)$,

$$\begin{aligned} Ug(x,m) &= U_s g(x,m) + U_r g(x,m) \\ &= U_s(g^*(x) + \sum_{j=1}^{k} f_j(m) \int_M g(x,m)\bar{f}_j(m) d\mu(m)) \\ &\quad + \int_0^1 \exp(i2\pi\alpha) dE(\alpha) g(x,m) \\ &= g^*(x) + \sum_{j=1}^{k} \lambda_j f_j(m) g_j(x) + \int_0^1 \exp(i2\pi\alpha) dE(\alpha) g(x,m). \end{aligned}$$

where E is a complex continuous spectral measure on L^2. We have

$$v_x^n(m) = U_s^n v_x = v^*(x) + \sum_{j=1}^{k} \lambda_j^n f_j(m) s_j(x) + \int_0^1 \exp(i2\pi\alpha) dE(\alpha) v(x,m), \quad (15)$$

where

$$s_j(x) = \int_M v(x,m) \bar{f}_j(m) d\mu(m).$$

Clearly, $s_j(x)$ could be considered as shape functions. The amplitudes $\lambda_j^n = \exp(i2\pi n\omega_j)$ oscillate in time. Note that the m dependence in the formulas above is due to the initial conditions m on the attractor. Since the spectrum of

U_r is continuous, the part $v_x|_{H_1}$ could be considered as the deterministic part of the field v_x., while $v_x|_{H_2}$ could be modeled by a stochastic process.

The functions $s_j(x)$ can in principle be determined from the foregoing discussion by determining U from the evolution equation (12) and finding its eigenvalues. However, this would be hard given that numerical solutions of (12) can be expensive and finding eigenvalues would generally require starting the simulation from various initial conditions on the attractor M. Another problem is that we would like to extract $v_x|_{H_1}$ from experimental data as well, but preparing experiments with various initial conditions on the attractor is all but impossible. Fortunately, there is a more direct way of obtaining this information, starting from the observation that the projection of the function v_x on the j-th eigenspace can be obtained as [17]

$$P_T^{\omega_j}(v_x(m)) = \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} e^{i2\pi k\omega_j} v_x(T^k(m)) = z(x) f_j(m). \tag{16}$$

Now,

$$\int_M v_x(m) \bar{f}_j(m) d\mu(m) = \int_M z(x) f_j \bar{f}_j d\mu = z(x) = s_j(x),$$

where the fact that the modulus of f_j is 1 was used. Since in applications we will not know $f_j(m)$ we can take the whole projection obtained in (16) and orthonormalize the resulting set.

Note that the decomposition (15) of the field v_x^n is reminiscent of the so-called "triple decomposition" [22], where a turbulent flow field is decomposed into its "mean", "periodic" and "fluctuating" component. The periodic component is extracted using the so-called "phase averaging" process. Define the following periodic mean of the sequence $v^n(x, m)$:

$$v_p(n, x, k, m) = \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N-1} v^{n+jk}(x, m).$$

Clearly, $v_p(n, x, k, m)$ is periodic in time with period k. Thus,

$$v_p(n, x, k, m) = \sum_{j=-k}^{k} v_k^j(x, m) e^{i2\pi nj/k},$$

where

$$
\begin{aligned}
v_k^t(x,m) &= \sum_{l=-k}^{k} v_p(l,x,k)e^{i2\pi tl/k} \\
&= \sum_{l=-k}^{k} \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N-1} v^{l+jk}(x,m)e^{i2\pi tl/k} \\
&= \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N-1} \sum_{l=-k}^{k} v^{l+jk}(x,m)e^{i2\pi tl/k} \\
&= \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N-1} \sum_{l=-k}^{k} v^{l+jk}(x,m)e^{i2\pi t(l+jk)/k} \\
&= \lim_{N\to\infty} \frac{1}{N} \sum_{j=0}^{N-1} v^{j}(x,m)e^{i2\pi jt/k} = v^*_{t/k}(x,m)
\end{aligned}
\tag{17}
$$

The above calculation shows that the computation of the so-called "periodic mean" with period k is equivalent to computing part of the field that corresponds to frequencies $j/k, j \in \{-k,k\}/\{0\}$:

$$
v_p(n,x,k,m) = \sum_{j=-k}^{k} v^*_{j/k}(x,m)e^{i2\pi nj/k}.
$$

Thus, $v_p(n,x,k)$ is the part of the field that oscillates in time with period k. This motivates a more general definition:

$$
v_p(n,x,\omega,m) = \sum_{\substack{j=-\infty \\ j\neq 0}}^{\infty} v^*_{j\omega}(x,m)e^{i2\pi nj\omega},
$$

where ω is an arbitrary number between $[0,1]$ and we subtracted the $j=0$ pert, since that corresponds to the time average and we include it separately in the next subsection. Since there is only a countable number of ω's for which $v_p(n,x,\omega,m) \neq 0$ [2], arranging the ω 's for which $v_p(n,x,\omega,m) \neq 0$ in a sequence $\{\omega_j, j \in \mathbb{Z}\}$, we define

$$
v_{ap}(n,x,m) = \sum_{\omega_j \neq 0} v_p(n,x,\omega_j,m).
$$

It should be clear that the zero-mean field $v_{ap}(n,x,m)$ is almost periodic in the sense of Bohr in the variable n [2]. Thus, we can call $v_{ap}(n,x,m)$ the *almost periodic mean* of the field v.

[2] This is the consequence of the fact that, for measure-preserving transformations, the harmonic averages (16) can only be non-zero for a countable set of ω [29].

The dependence of $v_{ap}(n,x,m)$ on m indicates that while a process might be ergodic, it could still retain some memory of the initial condition through the "phase" of the almost periodic part.

3.3 Dynamics on the attractor and the almost periodic mean

Now we can relate $v_{ap}(n,x,m)$ to the phase-space properties on the attractor of the dynamical system (12). Recall that existence of a factor $S : B \to B$ of T on $A \subset M$ is established by proving that there is a measurable *factor map* $F : A \to B$ such that $F \circ T = S \circ F$ a.e. and $\mu(F^{-1}(E)) = \nu(E)$ for all measurable $E \subset B$, and measures μ, ν, where T preserves μ and S preserves ν [19]. We have the following [17]:

Proposition 3 *Let $h_\omega : A \to \mathbb{C}$ be a non-constant eigenfunction of U associated with the eigenvalue $e^{-i2\pi\omega}$. Then h_ω is a factor map and T has a factor that is a rotation on a circle by angle $2\pi\omega$. Conversely, if T admits a factor map to rotation on the circle by angle $2\pi\omega$ then there is an eigenfunction of U associated with eigenvalue $e^{-i2\pi\omega}$.*

The meaning of this result is that, whenever there is a nonzero, quasi-periodic part of the field $v_p(n,x,\omega)$, there is a periodic or quasi-periodic rotation that is part of the motion on the attractor. In fact, since eigenfunctions define invariant partitions, this can be visualized as sets of initial conditions that are transported by the dynamics between sets of an invariant partition (see section 2).

The composite picture that arises from the above considerations is that the following "triple decomposition" arises from the spectral properties of the Koopman operator:

$$v(n,x,m) = v^*(x) + v_{ap}(n,x,m) + v_c(n,x,m),$$

where $v^*(x)$ is the time-averaged part of the field, $v_{ap}(n,x,m)$ is almost-periodic in time, and $v_c(n,x,m)$ is the part of the field that is genuinely aperiodic (or chaotic) in time. Thus, this part could be modelled as a stochastic process. This stochastic process can be expanded into Karhunen-Loeve modes in space (Proper Orthogonal Decomposition (POD), see [14]). In fact, since the modal dynamics of the POD in this case has continuous spectrum, one could expect that it might be hyperbolic. The finite-dimensional truncations should have good structural stability properties in this case.

A direct correspondence between various types of attractors studied in dynamical systems and the above decomposition can be drawn: quasi-periodic attractors correspond to decomposition $v(n,x,m) = v^*(x) + v_{ap}(n,x,m)$, skew-periodic attractors [6] correspond to decomposition $v(n,x,m) = v^*(x)+v_{ap}(n,x,m)+v_c(n,x,m)$, while Axiom A attractors [31] correspond to decomposition $v(n,x,m) = v^*(x) + v_c(n,x,m)$.

Example 4 *An example that nicely reveals the nature of the spectral decomposition described above is provided by the field defined on* $A = \{1, 2\}$ *as:*

$$\begin{aligned} v^n(1) &= \cos(2\pi\omega n) + \xi_1(n), \\ v^n(2) &= \sin(2\pi\omega n) + \xi_2(n), \end{aligned}$$

where $\xi_1(n)$ *and* $\xi_2(n)$ *are possibly correlated random processes of mean zero and possibly different variances, and* ω *is irrational. The correlation matrix for this field is given by*

$$\begin{pmatrix} \lim_{n\to\infty} \frac{1}{n}\sum_{j=0}^{n-1} v^j(1)v^j(1) & \lim_{n\to\infty} \frac{1}{n}\sum_{j=0}^{n-1} v^j(1)v^j(2) \\ \lim_{n\to\infty} \frac{1}{n}\sum_{j=0}^{n-1} v^j(2)v^j(1) & \lim_{n\to\infty} \frac{1}{n}\sum_{j=0}^{n-1} v^j(2)v^j(2) \end{pmatrix} = \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix},$$

where

$$\begin{aligned} c_1 &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} (\cos^2(2\pi\omega j) + \xi_1^2(j)) = \frac{1}{2} + \sigma_1, \\ c_1 &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} (\sin^2(2\pi\omega j) + \xi_2^2(j)) = \frac{1}{2} + \sigma_2, \end{aligned}$$

where σ_1, σ_2 *are variances of* ξ_1, ξ_2*, respectively. The orthonormal eigenvectors of this matrix are clearly* $(1, 0)$ *and* $(0, 1)$*. Assuming say* $c_1 > c_2$*, the energy contained in the first POD mode is* c_1*. The total energy is* $c_1 + c_2$*. It is easy to see that* $v_{ap}(n) = \cos(2\pi\omega n), \sin(2\pi\omega n)$*. This is a "travelling wave" mode and is not of the type* $f(n)\phi(x), n \in \mathbb{Z}, x \in A$*. In figure 3 we show the phase portrait of these processes, for*

$$\begin{aligned} v(1) &= \cos(2\pi n\sqrt(2)) + 0.3 * (u - 0.5), \\ v(2) &= \sin(2\pi n\sqrt(2)) + 0.2 * (u - 0.5), \end{aligned}$$

where u *is uniformly distributed on* $[0, 1]$*. The blue dots show the evolution of the field. Red dots represent projection on* $(1, 0)$ *(the first POD mode). Black dots represent evolution of the almost periodic component of the field* $(\cos(\omega n), \sin(\omega n))$

4 Model validation

The fact that, of all finite-dimensional linear projections, the Proper Orthogonal Decomposition is the one that contains, on average, most of the energy [14] is a noted and desirable property of POD. Energy is however, only one observable on the phase space of the system. In this section, following [17] we investigate a more general question of model validation and review some results that lead to suggestions on using energy and certain derived quantities as a basis for comparison between the projection and the "true" system. In addition we argue that phase information can be compared in a similar way.

The following result is useful in the context of comparing projections with the full dynamics [17]:

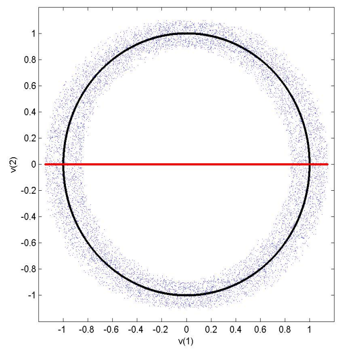


Figure 3: Evolution of the field in the equation (18) and its projections. Blue dots represent the evolution of the field. Red dots represent projection on $(1,0)$ (the first POD mode). Black dots represent evolution of the almost periodic component of the field $(\cos(2\pi\omega n), \sin(2\pi\omega n))$

Theorem 5 *Let M be a compact Riemannian manifold of dimension m. Let $l/2 > |f|$ and $\kappa_i, i \in \mathbb{N}^+$ a sequence of continuous periodic functions in $C([-l/2, l/2])$ that is complete. Consider a countable set of functions $f_{i_1,\ldots,i_{2m+1}} = \kappa_{i_1}(f) \cdot \kappa_{i_2}(f \circ T) \cdot \ldots \cdot \kappa_{i_{2m+1}}(f \circ T^{2m})$ (where $i_1, i_2, ..., i_{2m+1} \in \mathbb{N}^+$). Then, for $C^r, r \geq 1$ pairs (f, T) it is a generic property that the ergodic partition of a dynamical system T on M is*

$$\zeta_e = \bigvee_{i_1,\ldots,i_{2m+1}} \zeta_{f_{i_1,\ldots,i_{2m+1}}}.$$

The essence of the above result is the following. By Takens theorem, we know that we can embed the signal $f(T^j), j \in \mathbb{Z}^+$ of a continuous observable f of a system T into an $2m+1$ dimensional box $\mathbb{B}$ of side l, where $|f| < l/2$. It can be shown [17] that to find the ergodic partition we only need to exhibit a dense countable subset of continuous functions. Such a subset is going to be provided by products of compositions of $(2m+1)-$products of complete set of continuous periodic functions on $\mathbb{R}$ of period l with a generic observable f, i.e. we only need to compute the time-averages of functions

$$\kappa_{i_1}(f(x)) \cdot \kappa_{i_2}(f \circ T(x)) \cdot \ldots \cdot \kappa_{i_{2m+1}}(f \circ T^{2m}(x)).$$

Example 6 *The set of products of functions $\sin(\frac{2\pi}{l} ny), \cos(\frac{2\pi}{l} ky), \frac{1}{2}, y \in \mathbb{R}, k, l, n \in \mathbb{N}^+$ is a complete set in $C(\mathbb{B})$. If $m = 1$ (i.e the embedding dimension is 3), we should compute time averages of products*

$$f_1(\frac{2\pi}{l} nf(T^2x))f_2(\frac{2\pi}{l} kf(Tx))f_3(\frac{2\pi}{l} jf(x)),$$

where $f_i(z) = \sin(z)$, or $\cos(z)$ and $k, n, j \in \mathbb{N}^+$.

Theorem 5 can be used to identify invariant sets (and ultimately the ergodic partition) of a system without measuring all of its variables for all time. All that is needed is knowledge of initial conditions and knowledge of a single variable time trace [17].

According to the above description, the asymptotic dynamics partitions the phase space into invariant sets. A sequence of numbers $f^*_{i_1,\ldots,i_{2m+1}}$ is associated with each set in the partition. We can use time averages to compare systems as is done in the case of the Proper Orthogonal Decomposition. In that context, let $\phi_i(x), i = 1, ..., k$ be the first k modes of the projection and $a_i(n), i = 1, ..., k$ the associated amplitudes. The energy contained in the first n modes is given by

$$E_n = \lim_{n\to\infty} \frac{1}{n} \sum_{n=0}^{n-1} \sum_{i=1}^{k} a_i(n)\bar{a}_i(n)$$

is maximal with respect to all linear projections on k modes [14]. This of course does not mean that the projection of the "real" process on the phase space of the first k modes and the truncated "time-evolution" are the same, or even close. This is clearly indicated in example 4 and figure 3. However, Theorem 5 does indicate that using a single observable, two processes can be compared by combining that observable with a certain set of basis functions on an interval and taking finite products of the quantities obtained. In the context of chaotic dynamical systems the probabilistic approach is often taken and a system is described in terms of a histogram of a specific function g on the phase space. Let b be the bin size for the histogram and $z_j \in \mathbb{R},\ j \in \mathbb{Z}$ a sequence of numbers such that $z_{j+1} = z_j + b$. By the histogram we mean a step function, constant on every interval $I_j = (z_j - b/2, z_j + b/2]$:

$$H^T_g(I_j, x) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} \kappa_j \circ g(T^i(x)) = \kappa^*_j(x),$$

where $x \in M$. $H^T_g(I_j, x)$ tells us the proportion of time the time-series spends in the interval I_j. The function κ_j is the characteristic function on the interval $I_j = (z_j - b/2, z_j + b/2]$, i.e. $\kappa_j(u) = 1$ if $z_j - b/2 < u \leq z_j + b/2$ and zero otherwise. If T is ergodic, H is the same function for almost every initial condition x. Let $g(T^j_1)$ being the signal of the observable g produced by the full system and $g(T^j_2)$ signal of the observable g produced by a finite-dimensional projection. A possible pseudometric, if T_1, T_2 are ergodic, would be

$$d(T_1, T_2) = \sum_j w_j [H^{T^1}_g(I_j) - H^{T^2}_g(I_j)]^2,$$

where w_j is the weight that we put on comparison in interval, j the sum is over some finite set of j's.

The lesson learned from the rigorous study is that we should take time-averages (i.e. histograms) of products of $(\kappa_j \circ g(T^i(x))$ where $i = 0, ..., 2m$, and include them into the pseudometric. In this context we need to determine the

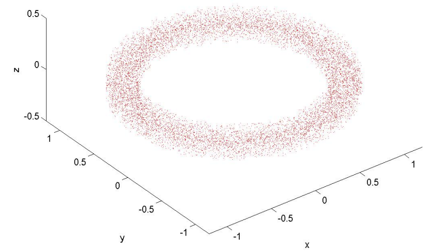


Figure 4: Evolution of the field in the equation (18).

dimensionality m of the system using the appropriate embedding theorem, say Takens. But our study in this paper suggests that a more appropriate procedure might to choose $m = p + s$ where p is the number of linearly independent frequencies in the almost periodic mean, and s the number of POD modes that we choose to represent the part of the process with continuous spectrum. In this case, we will obtain a process in $\mathbb{R}^{p+s}$ that will represent stochastic dynamics normal to a p-dimensional torus. In Example 4 we plotted the case $n = 1$ in figure 3 and the dynamics is seen to be stochastic around a 1-D circle. Consider the case of a process given by

$$\begin{aligned} v(1) &= \cos(2\pi n\sqrt{(}2)) + 0.3(u_1 - 0.5), \\ v(2) &= \sin(2\pi n\sqrt{(}2)) + 0.2(u_2 - 0.5), \end{aligned}$$

where u_1, u_2 are independent and uniformly distributed on $[0, 1]$. There are 2 independent stochastic directions (corresponding to 2 independent random variables that can be represented by 2 POD modes). In this case, $n = 1, k = 2$ and the phase portrait is shown in figure 4. We set $r = 1 + 0.3(u_1 - 0.5), z = 0.2(u_2 - 0.5), \theta = 2\pi n\sqrt{(}2)$ and $x = r\cos(\theta), y = r\sin(\theta)$.

In the case of our example 4 we could pursue such comparison by using the Haar basis on the interval $[-1, 1]$. We would compute the products of time-averages of the composition of elements of the basis with the energy time-series in the following way:

$$E^*_{jk} = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} \kappa_j(v^2(i)) \cdot \kappa_k(v^2(i-1)).$$

If $\kappa_j = \kappa_k = 1$, constant on $[-1, 1]$, $E_{1,1}$ is just the total average energy of the process. But all the numbers E^*_{jk} should be considered in order to compare the process with its projections. In the example 18 the projection onto the almost periodic part of the field clearly does much better in this sense than POD. It is interesting to note that the energy function is not generic in the sense of Takens, since only the absolute values of the projection amplitudes matter. More generally, the phase of the process is not of importance in calculating energy. Thus, the pseudometrics of time-averaging type are still not entirely satisfactory, as they loose all the "timescale" information about the system. For example, all of the irrational rotations on the circle are identified. To treat this problem, we need to extend our formalism to include additional information, as done in [17] for the case of harmonic averages.

5 Discussion and conclusions

There has been a substantial interest recently in improving the projection methods for obtaining low-dimensional models of formally infinite-dimensional systems by introducing stochastic terms to account for neglected modes [13, 7, 28, 21, 4, 15, 8] . A dynamical systems perspective on such modelling is provided in the work of Dellnitz and collaborators [10, 9] in the context of Perron-Frobenius operator for stochastic systems. Here we used the formalism for spectral properties of dynamical systems developed in [17] in the context of Koopman operator to discuss properties of finite-dimensional projections. The key observation is that the dynamics on the attractor can be split into an almost periodic part and a part that has continuous spectrum. The almost periodic part of the Koopman operator leads naturally to the definition of the almost periodic mean of the process. The rest of the field has continuous spectrum. Such a decomposition is often sought in turbulence studies [22, 11]. The decomposition presented here has a close relationship with the "triple decomposition" of [22]. It would be interesting to pursue ideas along these lines using the wavelet, instead of Fourier spectrum, given the success of the decomposition applied in [11]. These concepts might help in understanding e.g. in processes containing abundance of oscillatory phenomena on various time-scales in climate dynamics (see e.g. [25]). We tried to compare the properties of the Proper Orthogonal decomposition with the spectral decomposition proposed here. We argue that it is useful to apply the spectral decomposition first, to extract the almost periodic part of the field. The rest of the field has continuous spectrum. We speculate that applying POD to it should typically produce a finite-dimensional, hyperbolic system. Given the robustness of statistical properties of such systems to perturbations, finite dimensional truncations should do well in this case.

Attractors with mixed spectrum can be related to a symmetry in the system [6]. Proper Orthogonal Decomposition has been analyzed utilizing symmetry reduction ideas from geometric mechanics in [24]. It would be interesting to explore connections between the spectral ideas presented here and symmetry reduction further.

We have also discussed the issue of comparison of properties of finite-dimensional projections with the properties of the process they are modeling. Using the "statistical Takens theorem" proven in [17] we argued that comparison of average energy contained in the projection is one in the hierarchy of functionals of the field that need to be checked in order to assess the accuracy of the projection.

6 Appendix: Invariant and periodic partitions of the phase space

A partition ς of M is defined to be a collection of disjoint sets D^{ς}_{α}, where α is some indexing set, such that $\mu(\underset{\alpha}{\cup} D^{\varsigma}_{\alpha}) = \mu(M)$ (see [23]). A product $\varsigma \bigvee \lambda$ of two partitions ς, λ is a partition into sets $D^{\varsigma \bigvee \lambda}_{(\alpha,\beta)} = D^{\varsigma}_{\alpha} \cap D^{\lambda}_{\beta}$ i.e. sets that are intersections of elements of the two partitions. For a finite or countable product ζ of partitions ζ_i, we write $\zeta = \bigvee_i \zeta_i$.

If T is a dynamical system on M, then ς is an invariant partition for T provided that for any set $D_{\alpha_1} \in \varsigma, T^{-1}(D_{\alpha_1}) = D_{\alpha_2}, D_{\alpha_2} \in \varsigma$.

The key object in our considerations are partitions of the phase space into sets on which harmonic averages are constant, i.e. into level sets of f^*_{ω}. In particular, let f be a continuous function on M. The family of sets $C_{\alpha}, \alpha \in \mathbb{R}$ such that $C_{\alpha} = (f^*_{\omega})^{-1}(\alpha)$ is a (measurable) partition of M. We denote this partition by $\zeta_{f^*_{\omega}}$ and call it the *partition induced by* f under ω. Clearly, $\zeta_{f^*_{\omega}}$ is an invariant partition for T. An invariant partition ζ is called *periodic* under T with period p iff for any $C_{\alpha} \in \zeta$, $T^p C_{\alpha} = C_{\alpha}$.

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