Data-Driven Spectral Decomposition and Forecasting of Ergodic Dynamical Systems

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IPAM Workshop on Uncertainty Quantification for Multiscale Stochastic Systems and Applications
January 21, 2016
Setting & objectives

Ergodic dynamical system \((M, \mathcal{M}, \Phi_t, \mu)\) observed through a vector-valued function \(F : M \mapsto \mathbb{R}^n\).

Given time-ordered observations \(\{x_0, \ldots, x_{N-1}\}\) with \(x_i = F(a_i)\), we seek to perform

1. **Dimension reduction** with timescale separation and invariance under changes of observation modality
2. **Nonparametric forecasting** of observables on \(M\) with deterministic or statistical initial data
Outline

1. Representation of Koopman operators in a data-driven orthonormal basis
2. Time-change techniques
3. Modes of organized tropical convection

Acknowledgments
Tyrus Berry, John Harlim, Joanna Slawinska, Jane Zhao
State- and observable-centric viewpoints

- **State space viewpoint**
  In data space, we observe the manifold $F(M)$ and the vector field

  $$V|_x = \frac{dx}{dt} \quad \text{with} \quad x = F(\Phi_t a)$$

  Associated with the dynamical system is a group of unitary operators $U_t$ on $L^2(M, \mu)$ s.t.

  $$U_t f(a) = f(\Phi_t a)$$

  The generator $v$ of $\{U_t\}$ gives the directional derivative of functions along the dynamical flow

  $$vf(a) = \lim_{t \to 0} \frac{f(\Phi_t a) - f(a)}{t}, \quad V = DF v$$
Spectral characterization of ergodicity and mixing

A dynamical system \((M, M, \Phi_t, \mu)\) is called

- **Ergodic** if all \(\Phi_t\)-invariant sets have either zero or full measure

  **Spectral characterization:** 0 is a simple eigenvalue of \(v\) corresponding to a constant eigenfunction

- **Weak-mixing** if for all \(A, B \in M\) we have

  \[
  \lim_{t \to \infty} \frac{1}{t} |\mu(\Phi_t(A) \cap B) - \mu(A)\mu(B)| = 0
  \]

  **Spectral characterization:** 0 is the only eigenvalue of \(v\) and this eigenvalue is simple
Systems with pure point spectra

$L^2(M, \mu)$ has an orthonormal basis consisting of eigenfunctions of $\nu$

$$\nu(z) = \lambda z, \quad \lambda = i\omega, \quad \omega \in \mathbb{R}, \quad |z| = 1$$

The eigenvalues and eigenfunctions form a group

$$\nu(z\tilde{z}) = (\lambda + \tilde{\lambda})z\tilde{z}, \quad \nu(\tilde{z}) = \tilde{\lambda}\tilde{z}$$

- Such systems are metrically isomorphic to translations on compact Abelian groups equipped with the Haar measure

  The canonical phase spaces for diffeomorphisms of smooth manifolds are tori; constructions on other manifolds are available but have discontinuous eigenfunctions (Anosov & Katok 1970)
Dimension reduction for systems with pure point spectra

The group of eigenvalues for $M = \mathbb{T}^m$ is generated by $m$ rationally independent frequencies $\Omega_i \in \mathbb{R}$ with corresponding eigenfunctions $\zeta_i$

$$\omega_{k_1 \ldots k_m} = \sum_{j=1}^{m} k_j \Omega_j, \quad z_{k_1 \ldots k_m} = \prod_{j=1}^{m} \zeta_{j}^{k_j}, \quad k_j \in \mathbb{Z}$$

**Dimension reduction map.** $\pi : M \mapsto \mathbb{C}^m$ with

$$\pi(a) = (\pi_1(a), \ldots, \pi_m(a)) = (\zeta_1(a), \ldots, \zeta_m(a))$$

- The $\pi_i$ are **independent of observation modality**
- $\nu$ is **projectible** under $\pi_i$, and the system evolves as a simple harmonic oscillator in the image space

$$\frac{d\zeta_i(\Phi_t a)}{dt} = \nu(\zeta_i)(\Phi_t a) = i\Omega_i \zeta_i(\Phi_t a)$$
Vector field decomposition

Define the vector fields \( \nu_i : L^2(M, \mu) \mapsto L^2(M, \mu) \) through their action on the eigenfunctions:

\[
\nu_i(\zeta_1^{k_1} \cdots \zeta_i^{k_i} \cdots \zeta_m^{k_m}) = ik_i \Omega_i \zeta_1^{k_1} \cdots \zeta_i^{k_i} \cdots \zeta_m^{k_m}
\]

The \( \nu_i \) are linearly independent, nowhere vanishing, **mutually commuting** vector fields

\[
\nu = \sum_{i=1}^{m} \nu_i, \quad [\nu_i, \nu_j] = 0
\]

- Due to their vanishing commutator, the \( \nu_i \) can be thought of as **dynamically independent components**
- These vector fields can be realized in data space through the **pushforward map** \( DF : TM \mapsto T\mathbb{R}^n \)

\[
V_i = DF(\nu_i) = \nu_i(F) = \sum_k A_k \nu(z_k), \quad A_k = \langle z_k, F \rangle
\]
Data-driven basis

- Start from a **variable-bandwidth kernel** (Berry & Harlim 2014), $K_\epsilon : M \times M \mapsto \mathbb{R}_+$:

$$K_\epsilon(a_i, a_j) = \exp \left( -\frac{\|x_i - x_j\|^2}{\epsilon \hat{\sigma}_\epsilon(x_i)^{-1/m} \hat{\sigma}_\epsilon(x_j)^{-1/m}} \right),$$

$$m = \dim M, \quad x_i = F(a_i), \quad \hat{\sigma}_\epsilon(x_i) = \frac{1}{N(\pi \epsilon)^{m/2}} \sum_{j=0}^{N-1} e^{-\|x_i - x_j\|^2 / \epsilon},$$

- Apply the **diffusion maps normalization** (Coifman & Lafon 2006, Berry & Sauer 2015):

$$\hat{q}_\epsilon(a_i) = \frac{1}{N} \sum_{j=0}^{N-1} K_\epsilon(a_i, a_j), \quad \hat{K}_\epsilon'(a_i, a_j) = \frac{K_\epsilon(a_i, a_j)}{\hat{q}_\epsilon(a_j)}$$

$$\hat{d}_\epsilon(a_i) = \frac{1}{N} \hat{K}_\epsilon'(a_i, a_j), \quad \hat{p}_\epsilon(a_i, a_j) = \frac{K_\epsilon'(a_i, a_j)}{\hat{d}_\epsilon(a_i)}$$
Data-driven basis

- \( \hat{p}_\epsilon \) induces an **averaging operator** on \( L^2(M, \hat{\mu}) \) for the sampling measure \( \hat{\mu} = N^{-1} \sum_{i=0}^{N-1} \delta_{a_i} \):

\[
\hat{P}_\epsilon f(b) = \int_M \hat{p}_\epsilon(b, a) f(a) \, d\hat{\mu}(a) = \frac{1}{N} \sum_{j=0}^{N-1} \hat{p}_\epsilon(b, a_j) f(a_j)
\]

- By ergodicity, as \( N \to \infty \), \( \hat{P}_\epsilon f(b) \) converges \( \mu \)-a.s. to \( P_\epsilon f(b) \), where

\[
P_\epsilon f(b) = \int_M p_\epsilon(y, x) f(x) \, d\mu(x)
\]

is an averaging operator on \( L^2(M, \mu) \).
Data-driven basis

Uniformly on $M$ (Coifman & Lafon 2006),

$$P_\epsilon f(a) = f(a) + \epsilon \Delta f(a) + O(\epsilon^2),$$

where $\Delta$ is the **Laplace-Beltrami operator** associated with the Riemannian metric $h = \sigma^2/dg$

- Effect of variable-bandwidth kernel is a **conformal transformation** such that the Riemannian measure is equal to the invariant measure

- The eigenfunctions $\{\phi_0, \phi_1, \ldots\}$ of $\Delta$ are orthogonal on $L^2(M, \mu)$

- The **rescaled eigenfunctions** $\varphi_i = \phi_i/\eta_i^{1/2}$ corresponding to eigenvalue $\eta_i$ are orthogonal on $H^1(M, h)$

$$\int_M \text{grad}_h \varphi_i \cdot \text{grad}_h \varphi_j \, d\mu = \delta_{ij}$$

- In practice, we approximate $(\eta_i, \phi_i, \varphi_i)$ by solving for

$$\hat{P}_\epsilon \hat{\phi}_i = (1 - \epsilon \hat{\eta}_i)\hat{\phi}_i, \quad \hat{\phi}_i = \hat{\phi}_i/\hat{\eta}_i^{1/2}$$
Eigenvalue problem for the Koopman generator

\[ v(z) = \lambda z \]

- In dimension \( m \geq 2 \) the eigenvalues form a dense set on the imaginary line.
- We eliminate highly rough eigenfunctions by solving the eigenvalue problem for \( L_\epsilon = v + \epsilon \Delta \).

**Continuous problem.** Find \( z \in H^1(M, h) \) and \( \lambda \in \mathbb{C} \) s.t.

\[ \langle \psi, v(z) \rangle + \epsilon \langle \nabla_h \psi, \nabla_h z \rangle = \lambda \langle \psi, z \rangle, \quad \forall \psi \in H^1(M, h) \]

**Discrete approximation.** Set \( \hat{H}_l = \text{span}\{\hat{\varphi}_0, \ldots, \varphi_{l-1}\} \subseteq L^2(M, \hat{\mu}) \).
Find \( \hat{z} \in \hat{H}_l \) and \( \hat{\lambda} \in \mathbb{C} \) s.t.

\[ \langle \psi, \hat{v}(\hat{z}) \rangle_{\hat{\mu}} + \langle \nabla_h \psi, \nabla_h \hat{z} \rangle_{\hat{\mu}} = \hat{\lambda} \langle \psi, \hat{z} \rangle_{\hat{\mu}}, \quad \forall \psi \in \hat{H}_l. \]
Eigenvalue problem for the Koopman generator

\[
\langle \psi, \hat{v}(\hat{z}) \rangle_{\hat{\mu}} + \langle \text{grad}_h \psi, \text{grad}_h \hat{z} \rangle_{\hat{\mu}} = \hat{\lambda} \langle \psi, \hat{z} \rangle_{\hat{\mu}},
\]

\[
\hat{z} = \sum_{i=0}^{l-1} c_i \hat{\phi}_i, \quad \psi = \sum_{i=0}^{l-1} w_i \hat{\phi}_i
\]

- \( \hat{v} \) is a \textbf{finite-difference approximation} of \( v \), e.g.,

\[
\langle \psi, \hat{v}(\hat{z}) \rangle_{\hat{\mu}} = \sum_{i,j=0}^{l-1} w_i c_j \int_M \hat{\phi}_i \hat{v}(\hat{\phi}_j) d\hat{\mu}
\]

\[
= \sum_{i,j=0}^{l-1} w_i c_j \left[ \frac{1}{N} \sum_{k=1}^{N-2} \hat{\phi}_i(a_k) \frac{\hat{\phi}_j(a_{k+1}) - \hat{\phi}_j(a_{k-1})}{2 \delta t} \right]
\]

- By construction of the \( \{ \hat{\phi}_i \} \) basis,

\[
\langle \text{grad}_h \psi, \text{grad}_h \hat{z} \rangle_{\hat{\mu}} = \sum_{i,j=0}^{l-1} w_i c_j \delta_{ij}
\]

- Scheme remains well-conditioned at large spectral order \( l \)
Variable-speed flow on $\mathbb{T}^2$

\[ v = \sum_{\mu=1}^{2} v^\mu \frac{\partial}{\partial \theta^\mu} \]

\[ v^1 = 1 + \beta \cos \theta^1 \]

\[ v^2 = \bar{\omega} (1 - \beta \sin \theta^2) \]

\[ \bar{\omega} = \sqrt{30}, \quad \beta = \sqrt{1/2} \]
Results for variable-speed flow on $\mathbb{T}^2$

$\zeta_1$, $\Omega_1 = 0.71$

$\zeta_2$, $\Omega_2 = 3.87$
Results for variable-speed flow on $\mathbb{T}^2$

$\varsigma_1, \Omega_1 = 0.71$

$\varsigma_2, \Omega_2 = 3.87$

$V, V_1, V_2$
Forecasting densities and expectation values

The adjoint $U_t^*$ on $L^2(M, \mu)$ governs the evolution of probability densities relative to $\mu$

$$\rho_0 = \sum_k c_k(0) z_k, \quad c_k(0) = \langle z_k, \rho_0 \rangle, \quad k = (k_1, \ldots, k_m)$$

$$\rho_t = U_t^* \rho_0 = \sum_k c_k(t) z_k, \quad c_k(t) = \sum_k e^{-i\omega_k t} c_k(0)$$

The time-dependent expectation value of an observable $f$ is

$$\mathbb{E}_t f = \sum_k \hat{f}_k c_k^*(t), \quad \hat{f}_k = \langle z_k, f \rangle$$

- By computing $\mathbb{E}_t f$ and $\mathbb{E}_t f^2$ the method keeps track of both the forecast mean and the forecast uncertainty
- The forecast accuracy depends on the bandwidth of $f$ in the $\{z_k\}$ basis
Nonparametric forecasting of the variable-speed system on $\mathbb{T}^2$

Initial distribution has circular Gaussian density relative to $\mu$ with mean $(\pi, \pi)$ and variance $(30^{-1}, 30^{-1})$

Forecasts with the nonparametric model are in good agreement with ensemble forecasts with the perfect model for both the mean and uncertainty.
Time change and mixing

Given a flow $\Phi_t$ with generator $\nu$ and a positive function $f$, construct the flow $\Psi_t$ with generator $w = f^{-1} \nu$

$\Psi_t$ has the same orbits as $\Phi_t$, but evolves at different speed and has invariant measure $\nu$ with $d\nu = f \, d\mu$

- For any ergodic $\Phi_t$ there exists a time change s.t. $\Psi_t$ is mixing (Kochergin 1973)

Example on $\mathbb{T}^3$ (Fayad 2002). $\Phi_t$ is an irrational flow, and

$$f(\theta^1, \theta^2, \theta^3) = 1 + \Re \sum_{k=1}^{\infty} \sum_{|l| \leq k} \frac{e^{-k}}{k} \left( e^{ik\theta^1} + e^{ik\theta^2} \right) e^{ilz}$$
Regularization by time change

Construct an orthonormal basis for $L^2(M, \nu)$ with $d\nu = \|v\| d\mu$ using the kernel

$$K_\epsilon(a_i, a_j) = \exp \left( -\frac{\|x_i - x_j\|^2 \|V|_{x_i}|^{1/m} \|V|_{x_j}|^{1/m}}{\epsilon \sigma_\epsilon(x_i)^{-1/m} \sigma_\epsilon(x_j)^{-1/m}} \right)$$

Solve the eigenvalue problem

$$w(z) = i\omega z, \quad w = \frac{v}{\|v\|}, \quad z \in L^2(M, \nu)$$

- In the reduced coordinates $\pi(a) = z(a) \in \mathbb{C}$ the system evolves as an oscillator with **variable frequency** $\omega \|v\|

Make the vector field decomposition

$$v = \sum_{i=1}^{m} v_i, \quad v_i = \|v\| w_i, \quad w = \sum_{i=1}^{m} w_i, \quad [w_i, w_j] = 0$$

- In general, the $v_i$ are **non-commuting** vector fields
Flow on $\mathbb{T}^2$ with fixed points (Oxtoby 1953)

The system

$$v = \sum_{\mu=1}^{2} v^\mu \frac{\partial}{\partial \theta^\mu}$$

$$v^1 = \alpha(1 - \cos(\theta^1 - \theta^2)) + (1 - \alpha)(1 - \cos \theta^2)$$

$$v^2 = \alpha(1 - \cos(\theta^1 - \theta^2))$$

has a fixed point at $\theta^1 = \theta^2 = 0$, and preserves the Haar measure.
Vector field decomposition for the fixed-point system

\[ \zeta_1, \Omega_1 = 0.74 \]

\[ \zeta_2, \Omega_2 = 0.17 \]

\begin{align*}
\theta_2/\pi & \quad 0 & \quad 0.5 & \quad 1 & \quad 1.5 & \quad 2
\end{align*}

\begin{align*}
\theta_1/\pi & \quad 0 & \quad 1 & \quad 2 & \quad -1.5 & \quad 30 & \quad 40 & \quad t
\end{align*}

\begin{align*}
\text{Re}(z) & \quad -1 & \quad 0 & \quad 1 & \quad -1.5
\end{align*}

\begin{align*}
\text{Im}(z) & \quad 0 & \quad 0.5 & \quad 1 & \quad -1.5
\end{align*}
Vector field decomposition for the fixed-point system

\[ \zeta_1, \Omega_1 = 0.74 \]

\[ \zeta_2, \Omega_2 = 0.17 \]
Nonparametric forecasting
Analysis of organized tropical convection

- **Brightness temperature**, $T_b$, is the blackbody emission temperature received from Earth by satellites.
- Deep convective clouds become cold, and present as a negative $T_b$ anomaly against the Earth’s surface.
- We analyze $T_b$ data from the CLAUS archive averaged over the latitudes $15^\circ$S–$15^\circ$N.
- Sampling is $8 \times$ daily at $0.5^\circ$ resolution for the period 1983–2006.
Delay-coordinate embeddings

- The raw $T_b(t)$ timeseries is highly non-Markovian

- To recover information lost in partial observations, we perform delay-coordinate mapping (Packard et al. 1980, Sauer et al. 1991)

  $$x(t) = (T_b(t), T_b(t - \delta t), \ldots, T_b(t - (q - 1) \delta t))$$

- This procedure significantly improves the quality of the diffusion eigenfunction basis (G. & Majda 2012, Berry et al. 2013)

- We use $q = 512$, equivalent to 64 days (intraseasonal timescale)
Multiple timescales are resolved including:

- (a) The annual cycle.
- (b, c) Intraseasonal oscillations.
- (d, e) Convectively coupled equatorial waves (CCEWs).
Spatiotemporal reconstructions

- (b, f) Annual cycle.
- (c) Madden-Julian oscillation.
- (d,h) Westward-propagating CCEWs.
- (g) Boreal summer intraseasonal oscillation (Indian Monsoon).
Effects of partial observations

- The computed Koopman eigenfunctions have amplitude modulations which are not consistent with the skew-symmetry of $\nu$.
- Despite delay-coordinate mapping, it is unrealistic to expect that we have recovered the full attractor of the climate system.
- Instead of the full generator, it is more likely that we are approximating an operator of the form
  \[ \tilde{v} = \Pi \nu \Pi, \]
  where $\Pi$ is a projector to the subspace of the full $L^2$ space on the attractor spanned by the diffusion eigenfunctions obtained from $T_b$.
- It is plausible that an effective description of $\tilde{v}$ is through a nonautonomous advection-diffusion process.
- Consistent with stochastic oscillator models for the MJO (Chen et al. 2014).
Summary

- The spectral properties of Koopman operators have attractive properties for dimension reduction and nonparametric forecasting of dynamical systems.

- These operators can be approximated from time-ordered data with no a priori knowledge of the equations of motion using kernel methods.

- In systems with pure point spectra, the eigenfunctions of the Koopman group lead to a decomposition of the dynamics into a collection of independent harmonic oscillators.

- Time change extends the applicability of Koopman eigendecomposition techniques to certain classes of mixing systems, which are now decomposed into coupled oscillators with time-dependent frequencies.
References