Data-Driven Spectral Decomposition and Forecasting of Ergodic Dynamical Systems

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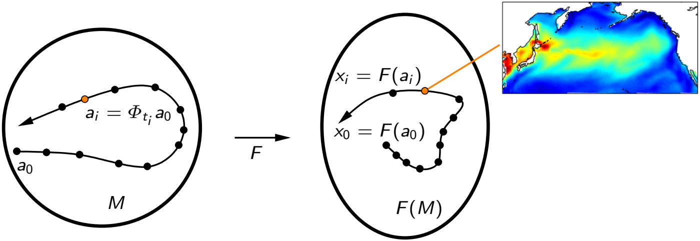
Setting & objectives



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 $\{x_0, \dots, x_{N-1}\}$ 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
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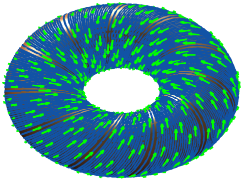
State- and observable-centric viewpoints

- **State space viewpoint**

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

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



- **Operator-theoretic viewpoint** (Mezić et al. 2004, 2005, 2012, ...)
  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 $(M, \mathcal{M}, \Phi_t, \mu)$ is called

- **Ergodic** if all Φ_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 $A, B \in \mathcal{M}$ 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 v

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

The eigenvalues and eigenfunctions form a group

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

- 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 ζ_i

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

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

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

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

$$\frac{d\zeta_i(\Phi_t a)}{dt} = v(\zeta_i)(\Phi_t a) = \mathrm{i}\Omega_i \zeta_i(\Phi_t a)$$

Vector field decomposition

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

$$v_i(\zeta_1^{k_1} \cdots \zeta_i^{k_i} \cdots \zeta_m^{k_m}) = \mathrm{i} k_i \Omega_i \zeta_1^{k_1} \cdots \zeta_i^{k_i} \cdots \zeta_m^{k_m}$$

The v_i are linearly independent, nowhere vanishing, **mutually commuting** vector fields

$$v = \sum_{i=1}^{m} v_i, \quad [v_i, v_j] = 0$$

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

$$V_i = DF(v_i) = v_i(F) = \sum_k A_k v(z_k), \quad A_k = \langle z_k, F \rangle$$

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 μ-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 Δ is the **Laplace-Beltrami operator** associated with the Riemannian metric $h = \sigma^{2/d} g$

- Effect of variable-bandwidth kernel is a **conformal transformation** such that the Riemannian measure is equal to the invariant measure
- The eigenfunctions $\{\phi_0, \phi_1, \dots\}$ of Δ are orthogonal on $L^2(M, \mu)$
- The **rescaled eigenfunctions** $\varphi_i = \phi_i / \eta_i^{1/2}$ corresponding to eigenvalue η_i are orthogonal on $H^1(M, h)$

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

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

$$\hat{P}_\epsilon \hat{\phi}_i = (1 - \epsilon \hat{\eta}_i) \hat{\phi}_i, \quad \hat{\varphi}_i = \hat{\phi}_i / \hat{\eta}_i^{1/2}$$

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.

$$\langle \psi, v(z) \rangle + \epsilon \langle \operatorname{grad}_h \psi, \operatorname{grad}_h z \rangle = \lambda \langle \psi, z \rangle, \quad \forall \psi \in H^1(M, h)$$

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

$$\langle \psi, \hat{v}(\hat{z}) \rangle_{\hat{\mu}} + \langle \widehat{\operatorname{grad}}_h \psi, \widehat{\operatorname{grad}}_h \hat{z} \rangle_{\hat{\mu}} = \hat{\lambda} \langle \psi, \hat{z} \rangle_{\hat{\mu}}, \quad \forall \psi \in \hat{H}_l.$$

Eigenvalue problem for the Koopman generator

$$\langle \psi, \hat{v}(\hat{z}) \rangle_{\hat{\mu}} + \langle \widehat{\operatorname{grad}}_h \psi, \widehat{\operatorname{grad}}_h \hat{z} \rangle_{\hat{\mu}} = \hat{\lambda} \langle \psi, \hat{z} \rangle_{\hat{\mu}},$$

$$\hat{z} = \sum_{i=0}^{l-1} c_i \hat{\varphi}_i, \quad \psi = \sum_{i=0}^{l-1} w_i \hat{\varphi}_i$$

- $\hat{v}$ is a **finite-difference approximation** of v, e.g.,

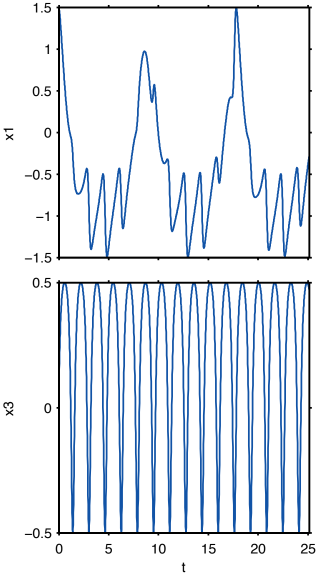
$$\begin{aligned} \langle \psi, \hat{v}(\hat{z}) \rangle_{\hat{\mu}} &= \sum_{i,j=0}^{l-1} w_i c_j \int_M \hat{\varphi}_i \hat{v}(\hat{\varphi}_j)\, d\hat{\mu} \\ &= \sum_{i,j=0}^{l-1} w_i c_j \left[\frac{1}{N} \sum_{k=1}^{N-2} \hat{\varphi}_i(a_k) \frac{\hat{\varphi}_j(a_{k+1}) - \hat{\varphi}_j(a_{k-1})}{2\,\delta t} \right] \end{aligned}$$

- By construction of the $\{\hat{\varphi}_i\}$ basis,

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

- Scheme remains well-conditioned at large spectral order l

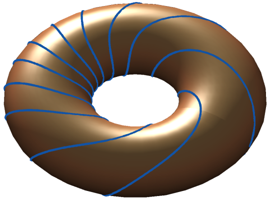
Variable-speed flow on $\mathbb{T}^2$



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

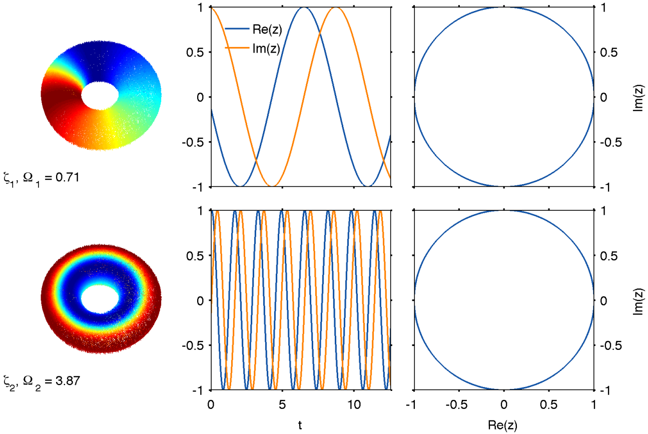
$$v^1 = 1 + \beta \cos \theta^1$$

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

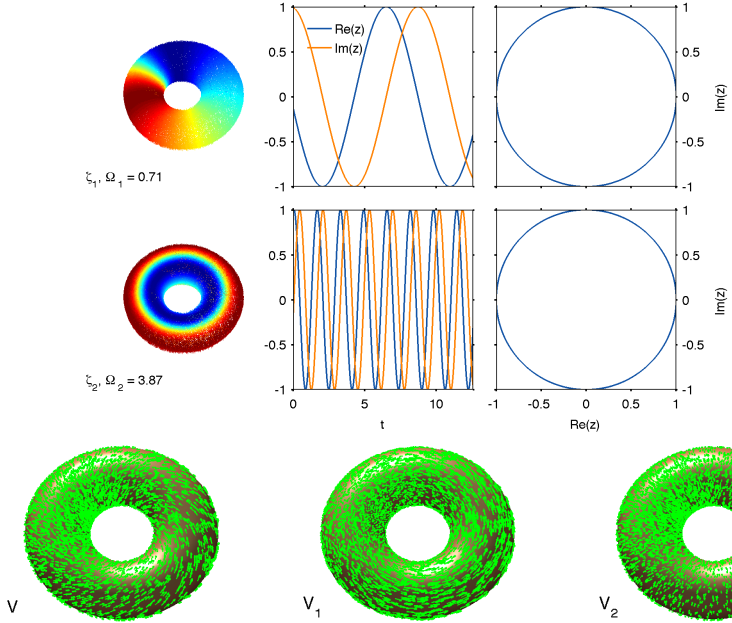


$\bar{\omega} = \sqrt{30}$, $\beta = \sqrt{1/2}$

Results for variable-speed flow on $\mathbb{T}^2$



Results for variable-speed flow on $\mathbb{T}^2$



Forecasting densities and expectation values

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

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

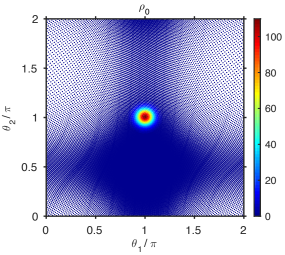
$$\rho_t = U_t^* \rho_0 = \sum_k c_k(t) z_k, \quad c_k(t) = \sum_k e^{-\mathrm{i}\omega_k t} c_k(0)$$

The time-dependent expectation value of an observable f is

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

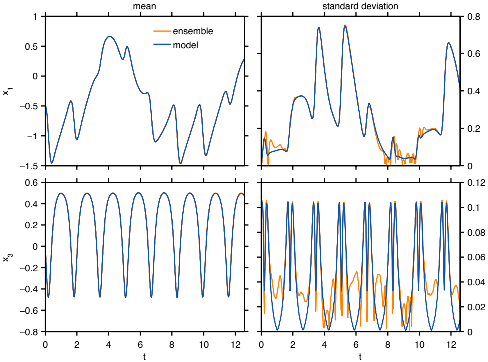
- By computing $\mathbb{E}_t f$ and $\mathbb{E}_t f^2$ the method keeps track of both the **forecast mean** and the **forecast uncertainty**
- The forecast accuracy depends on the **bandwidth** of f in the $\{z_k\}$ basis

Nonparametric forecasting of the variable-speed system on $\mathbb{T}^2$



Initial distribution has circular Gaussian density relative to μ with mean (π, π) 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

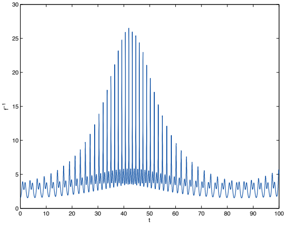


Time change and mixing

Given a flow Φ_t with generator v and a positive function f, construct the flow Ψ_t with generator $w = f^{-1} v$

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

- For any ergodic Φ_t there exists a time change s.t. Ψ_t is **mixing** (Kochergin 1973)



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

$$f(\theta^1, \theta^2, \theta^3) = 1 + \mathrm{Re} \sum_{k=1}^{\infty} \sum_{|l| \le k} \frac{e^{-k}}{k} \left(e^{\mathrm{i}k\theta^1} + e^{\mathrm{i}k\theta^2} \right) e^{\mathrm{i}lz}$$

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

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

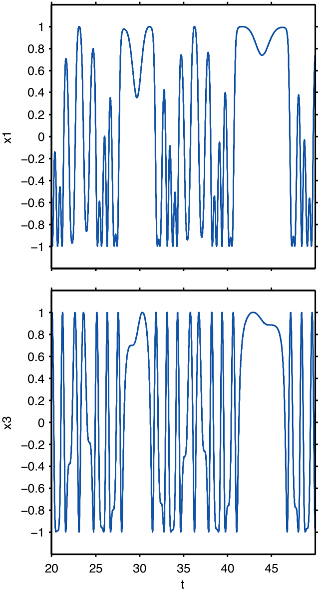
- In the reduced coordinates $\pi(a) = z(a) \in \mathbb{C}$ the system evolves as an oscillator with **variable frequency** $\omega\|v\|$

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

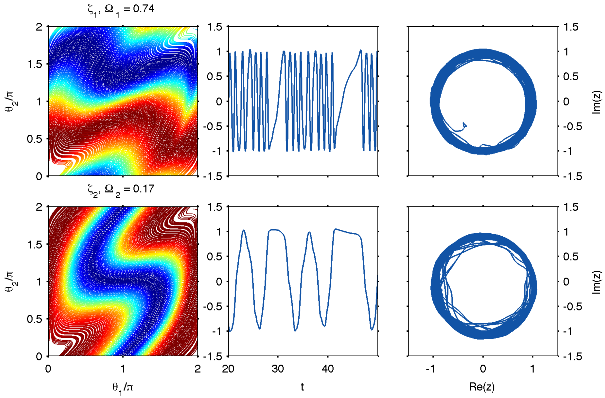
$$v = \sum_{\mu=1}^{2} v^\mu \frac{\partial}{\partial \theta^\mu}$$

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

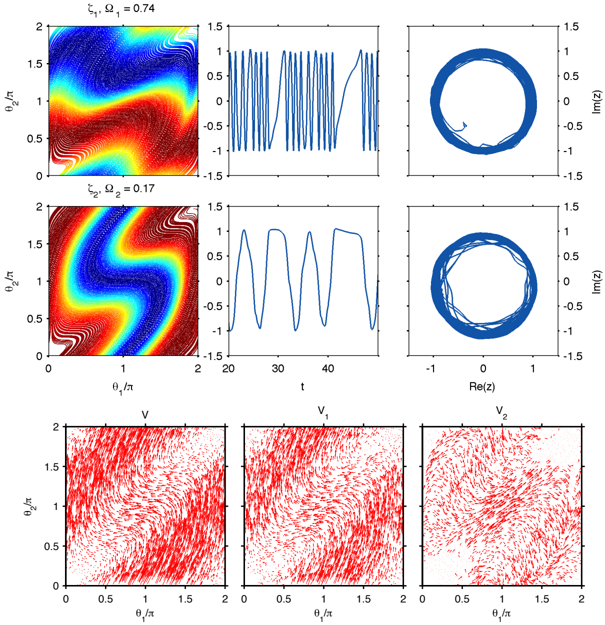
$$v^2 = \alpha(1 - \cos(\theta^1 - \theta^2))$$

has a fixed point at $\theta^1 = \theta^2 = 0$, and preserves the Haar measure

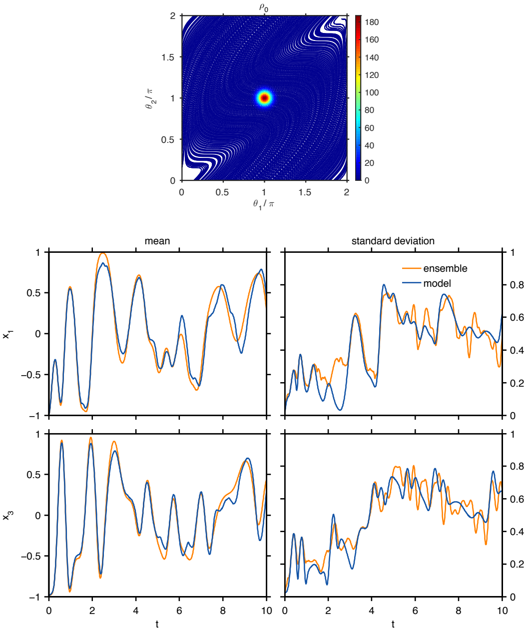
Vector field decomposition for the fixed-point system



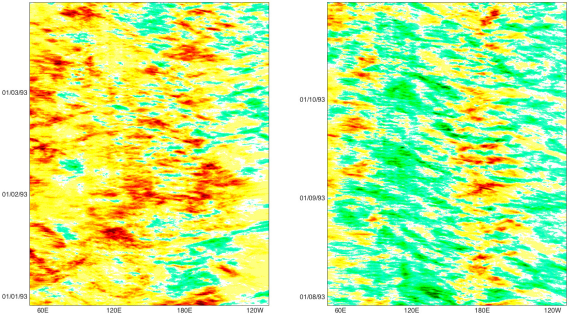
Vector field decomposition for the fixed-point system



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°S–15°N
- Sampling is 8 $\times$ daily at 0.5° resolution for the period 1983–2006

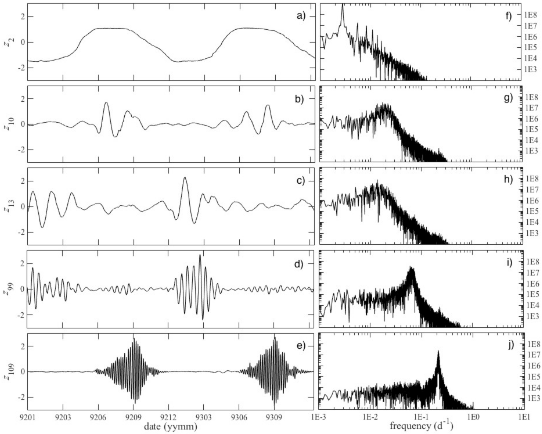
Delay-coordinate embeddings

- 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)

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

- 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)

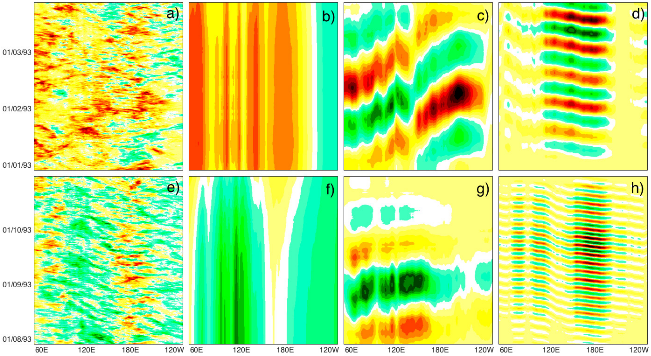
Koopman eigenfunctions



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 v
- 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

$$\tilde{v} = \Pi v \Pi,$$

  where Π 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

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