Operator-Theoretic Approaches for Coherent Feature Extraction in Complex Systems

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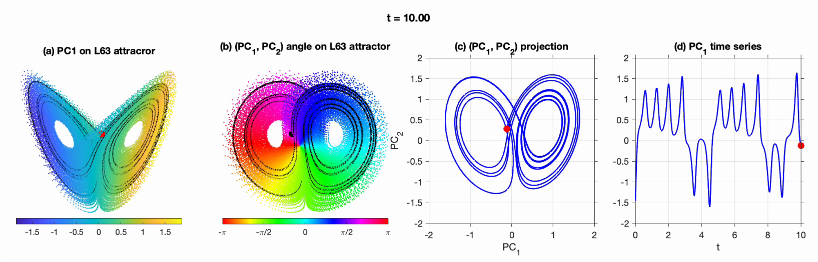
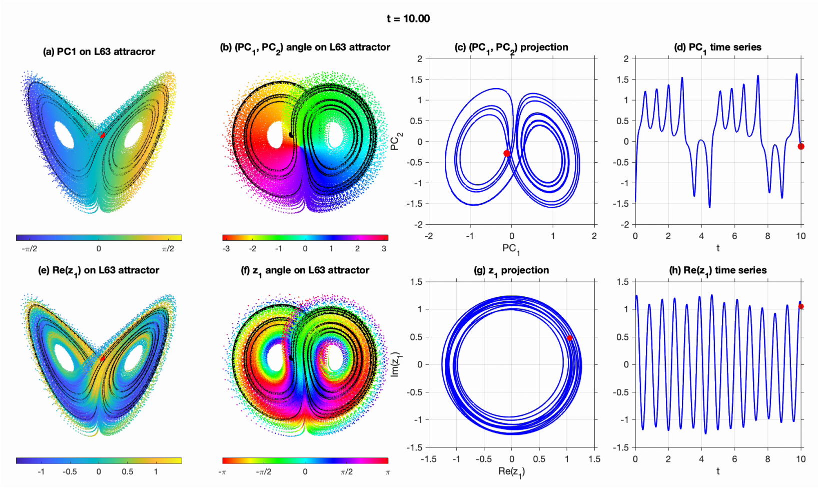
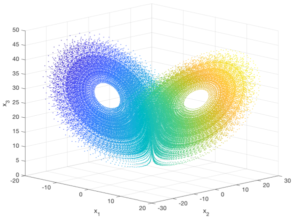

t = 10.00
(a) PC1 on L63 attracror
-1.5 -1 -0.5 0 0.5 1 1.5
(b) (PC1, PC2) angle on L63 attractor
-π -π/2 0 π/2 π
(c) (PC1, PC2) projection
PC2
PC1
-2 -1 0 1 2
(d) PC1 time series
0 2 4 6 8 10
t


t = 10.00
(a) PC1 on L63 attracror
(b) (PC$_1$, PC$_2$) angle on L63 attractor
(c) (PC$_1$, PC$_2$) projection
(d) PC$_1$ time series
(e) Re(z$_1$) on L63 attractor
(f) z$_1$ angle on L63 attractor
(g) z$_1$ projection
(h) Re(z$_1$) time series
-π/2
0
π/2
-3
-2
-1
0
1
2
3
-1
-0.5
0
0.5
1
-π
-π/2
0
π/2
π
PC$_1$
PC$_2$
t
Re(z$_1$)
Im(z$_1$)

Operator-theoretic description of dynamical systems



A dynamical flow $\Phi^t : X \to X$ acts on **spaces of observables** through intrinsically linear operators (**Koopman operators**):

$$\mathcal{F} = \{f : X \to \mathbb{C}\},$$
$$U^t : \mathcal{F} \to \mathcal{F}, \quad U^t f(x) = f(\Phi^t(x)).$$

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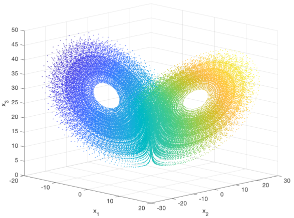

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$$f = g + h \implies U^t f(x)) = g(\Phi^t(x)) + h(\Phi^t(x)) = U^t g(x) + U^t h(x),$$
$$f = cg \implies U^t f(x) = f(\Phi^t(x)) = cg(\Phi^t(x)) = cU^t g(x).$$

Objectives

1. Identify **coherent observables** under the dynamics
   (spectral approximation of operators).
2. Perform **forecasting** of observables
   (pointwise approximation of operators).

- Methods should be **data-driven**, i.e., only utilize information from a time-ordered sequence of measurements.
- Challenges due to infinite dimensionality include the presence of **unbounded operators** and **continuous spectra**.

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- Operator-theoretic formalism originally introduced in the 1930s (Koopman 1931; von Neumann 1932).
- More recently, there has been significant interest in data-driven approaches (Dellnitz & Junge 1999; Dellnitz & Froyland 2000; Mezić & Banaszuk 2004; Mezić 2005; Rowley et al. 2009; Schmidt 2010; Froyland et al. 2014; Berry et al. 2015; Froyland 2015; G. et al. 2015; Williams et al. 2015; Klus et al. 2016; Brunton et al. 2017; Wu & Noé 2017; Korda et al. 2018; Das et al. 2019, 2020, 2021; G. 2019, 2021; Thiede et al. 2019; Alexander & G. 2020; Berry et al. 2020...).

Coherent observables through Koopman spectral analysis

A nonzero observable $z : X \to \mathbb{C}$ is said to be a **Koopman eigenfunction** if there exists $\lambda_t \in \mathbb{C}$ such that

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- Restrict attention to eigenfunctions $z \in L^2(\mu)$, where μ is an **invariant measure** of the dynamics.
- In that case, $\lambda_t = e^{i\omega t}$, where $\omega \in \mathbb{R}$ is an **eigenfrequency** of the dynamical system.
- Koopman eigenfunctions in measure-preserving systems form a distinguished class of observables evolving periodically under the dynamics at intrinsic frequencies, even if the flow map Φ^t is aperiodic:

$$U^t z = e^{i\omega t} z.$$

Example: Rectification of variable-frequency oscillator

$$\dot{\theta} = v(\theta) \equiv \alpha(1 + \beta \sin\theta),$$
$$\theta \in S^1, \quad \alpha > 0, \quad 0 \le \beta < 1$$

- Koopman eigenfunctions:

$$z_j(\theta) = e^{i\omega_j h(\theta)}, \quad \omega_j = \frac{2\pi j}{T}, \quad j \in \mathbb{Z},$$
$$h(\theta) = \int_0^\theta \frac{1}{v(\vartheta)}\, d\vartheta, \quad T = h(2\pi).$$

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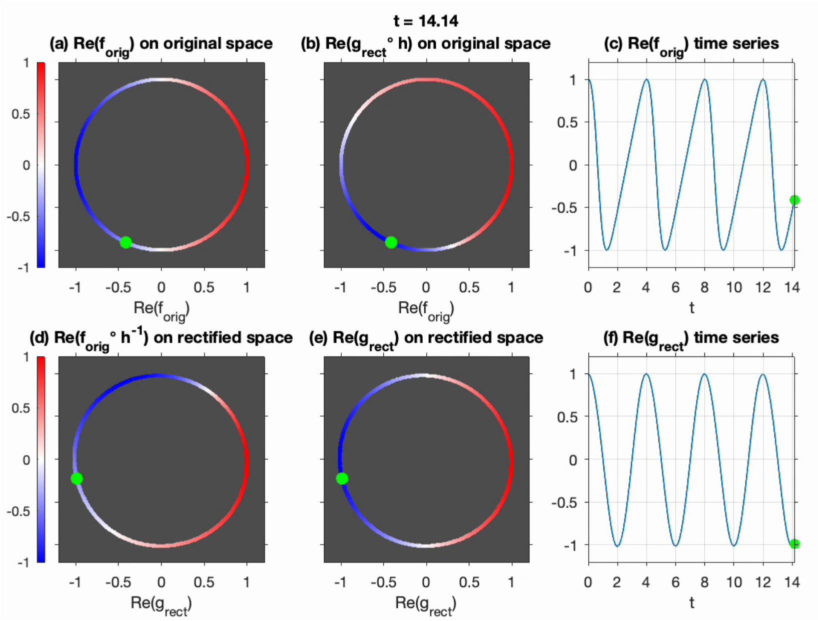
- Viewed as features $z_j : S^1 \to \mathbb{C}$, the Koopman eigenfunctions **rectify** the oscillation:

$$\begin{CD} S^1 @>{\Phi^t}>> S^1 \\ @V{z_j}VV @VV{z_j}V \\ \mathbb{C} @>{e^{i\omega_j t}\cdot}>> \mathbb{C} \end{CD}$$

Example: Rectification of variable-frequency oscillator



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An observable $z \in L^2(\mu)$ is said to be an **ϵ-approximate Koopman eigenfunction** if there exists $\nu_t \in \mathbb{C}$ such that

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- A Koopman eigenfunction is an ϵ-approximate eigenfunction for every $\epsilon > 0$.
- A natural notion of **coherence** is to require that z is an ϵ-approximate eigenfunction for "small" ϵ, and t lying in a "large" time interval.

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Given: Time series data $y_0, \dots, y_{N-1}$, with $y_n = F(x_n)$, of an observable $F : X \to \mathbb{R}^d$, sampled along a dynamical trajectory, $x_n = \Phi^{n\,\Delta t}(x_0)$.

1. Map the data into **delay-coordinate space**,

$$y_n \mapsto \tilde{y}_n = (y_n, y_{n-1}, \dots, y_{n-Q+1}) \in \mathbb{R}^{dQ}.$$

2. Introduce a **kernel function** $k_Q : \mathbb{R}^{dQ} \times \mathbb{R}^{dQ} \to \mathbb{R}$, and compute the associated $N \times N$ kernel matrix,

$$\boldsymbol{K}_Q = [k_Q(\tilde{y}_m, \tilde{y}_n)], \quad 0 \le m, n \le N - 1.$$

3. Compute eigenvalues and eigenvectors of $\boldsymbol{K}_Q$,

$$\boldsymbol{K}_Q \vec{\phi}_j = \lambda_j \vec{\phi}_j.$$

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Result [Das & G. 19; G. 21]**:** *For a suitable choice of kernel k_Q the following hold:*

1. *As $N \to \infty$, $\vec{\phi}_j \in \mathbb{R}^N$ converges to a continuous eigenfunction $\phi_j : X \to \mathbb{R}$ of a kernel integral operator K_Q on $L^2(\mu)$.*
2. *If the eigenvalue corresponding to ϕ_j is sufficiently isolated in the spectrum of K_Q, then the complex-valued observable $z = \phi_j + i\phi_{j+1}$ is an ϵ_t-approximate eigenfunction of U^t for a bound*

$$\epsilon_t \sim \frac{t}{\lambda_j Q}.$$

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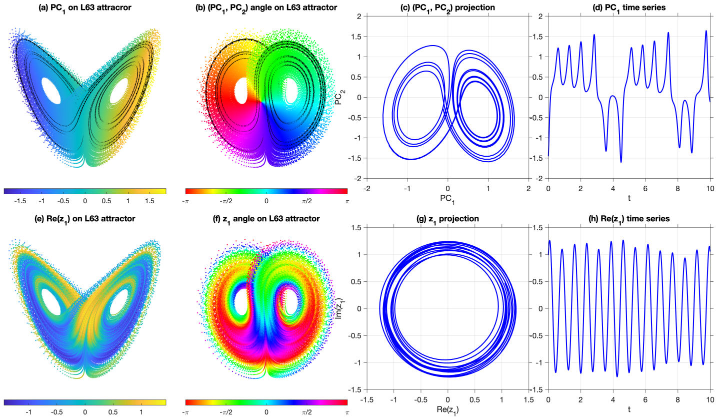

Galerkin approximation of the generator (G. et al. 17; G. 19; Thiede et al. 19)

$$V : D(V) \to L^2(\mu), \quad D(V) \subset L^2(\mu)$$

$$Vf = \lim_{t\to 0} \frac{U^t f - f}{t}, \quad V^* = -V, \quad U^t = e^{tV}$$

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- The matrix elements of the generator can be approximated in the kernel eigenfunction basis using **temporal finite differences**:

$$\begin{aligned}
\langle \phi_i, V\phi_j \rangle &= \int_X \phi_i(x) V\phi_j(x)\, d\mu(x) \\
&= \lim_{\Delta t\to 0} \lim_{N\to\infty} \frac{\vec{\phi}_i \cdot \boldsymbol{U}^{\Delta t} \vec{\phi}_j - \delta_{ij}}{N\,\Delta t} \\
&\approx \frac{1}{N\,\Delta t} \sum_{n=0}^{N-1} \phi_{n,i}(\phi_{j,n+1} - \phi_{j,n}).
\end{aligned}$$

Galerkin approximation of the generator (G. et al. 17; G. 19; Thiede et al. 19)

$$V_\epsilon z_j = \gamma_j z_j$$
$$V_\epsilon = V - \epsilon\Delta, \quad \epsilon > 0$$

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- Δ is a **diffusion operator**, constructed from the eigenvalues/eigenfunctions of the kernel integral operator:

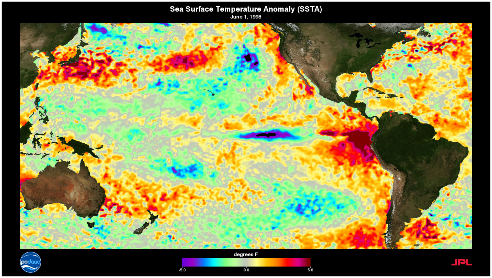
$$\Delta \phi_i = \eta_i \phi_i, \quad \eta_i = \frac{1}{\lambda_i} - 1, \quad i \in \{0, 1, \dots, \}.$$

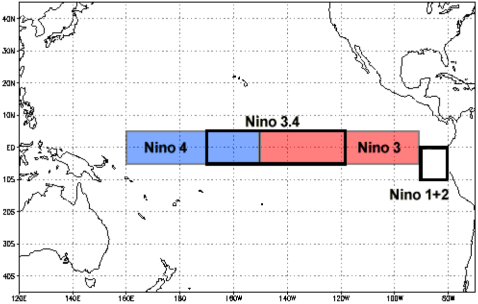
- The eigenvalue problem for the regularized generator V_ϵ is approximated by a matrix eigenvalue problem,

$$(\boldsymbol{V} - \epsilon \boldsymbol{\Delta}) \vec{z}_j = \gamma_j \boldsymbol{G} \vec{z}_j.$$

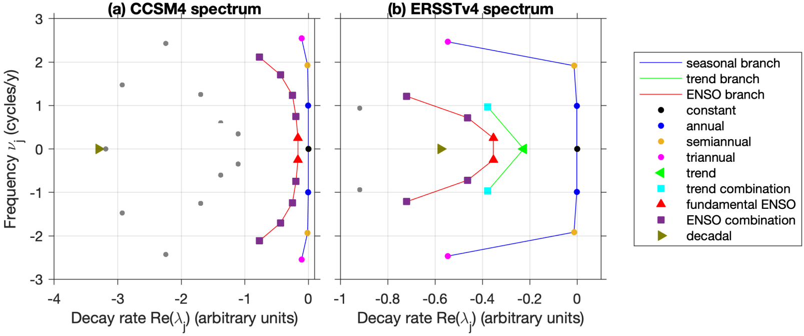
- $\operatorname{Im} \gamma_j$: Approximate Koopman eigenfrequency.
- $\operatorname{Re} \gamma_j$: Dirichlet energy (decay rate) of z_j.

El Niño Southern Oscillation (ENSO)

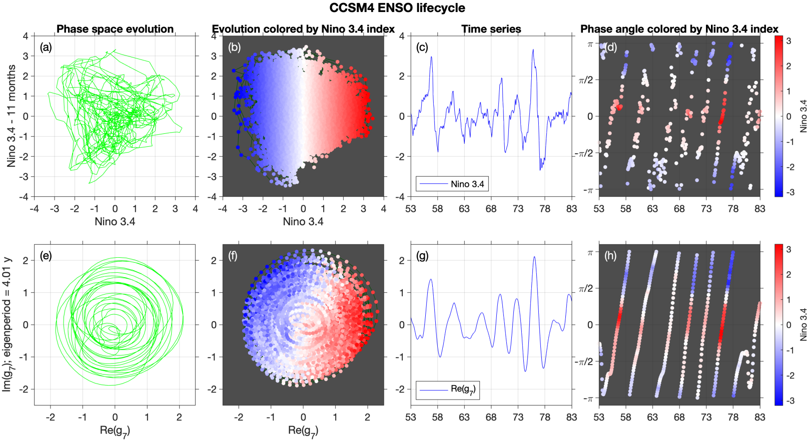




Koopman spectra in models and observations (Froyland et al. 21)



ENSO lifecycle recovered from approximate Koopman eigenfunctions



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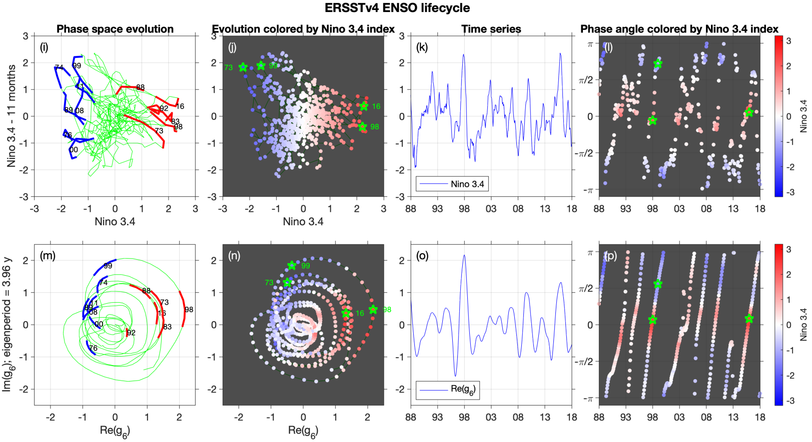

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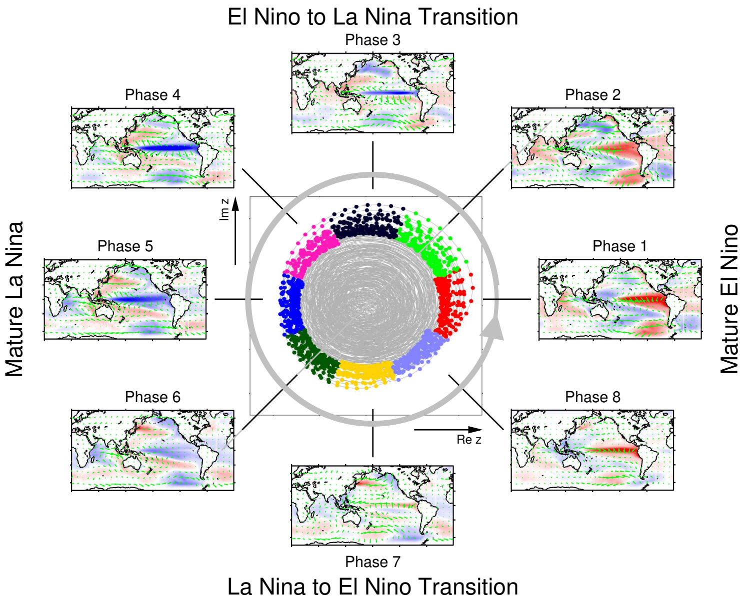

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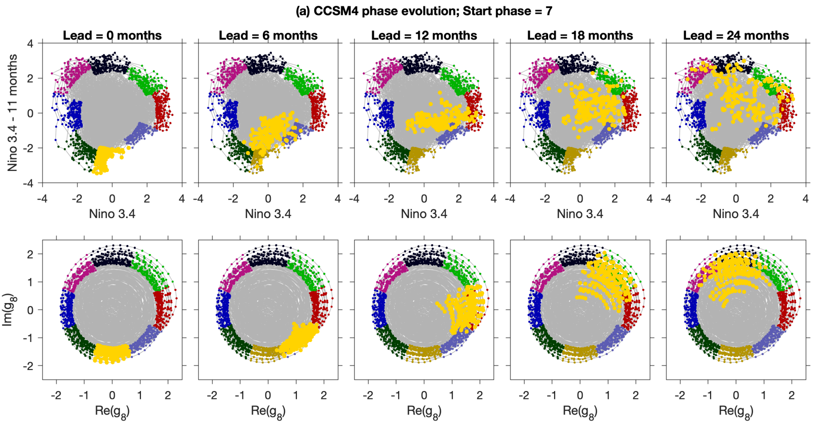
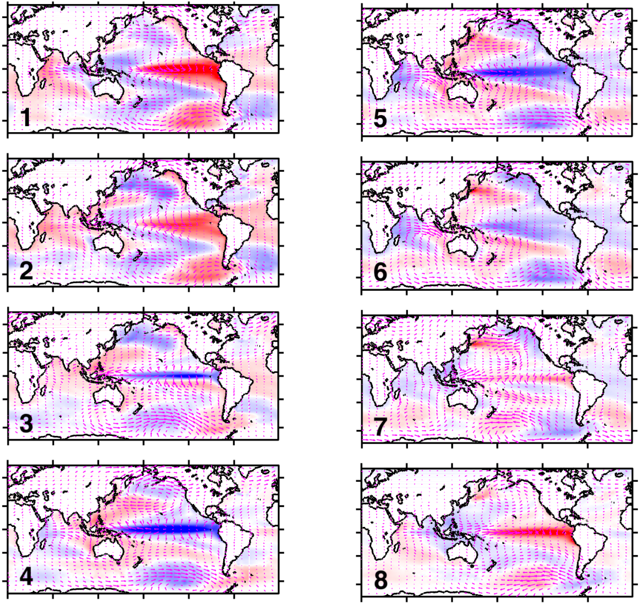


ENSO phase composites



Conclusions

- **Operator-theoretic approaches**, combined with **kernel methods for machine learning**, provide a useful route to identifying coherent observables of dynamical systems.
- Eigenfunctions of kernel integral operators constructed from **delay-coordinate-mapped data** identify ϵ-approximate eigenfunctions of Koopman operators with persistent cyclical behavior, potentially under mixing (chaotic) dynamics.
- Methods are **refinable**, in the sense of spectral convergence, as the amount of training data increases.
- V&V and UQ applications, including model intercomparisons and estimation of conditional statistics, are promising directions for future work.

References

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