# Reproducing Kernel Hilbert Space Approaches for Spectral Analysis of Dynamical Systems

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Operator Theoretic Methods in Dynamic Data Analysis and Control
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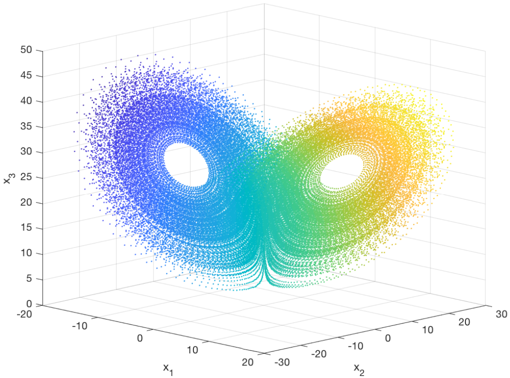
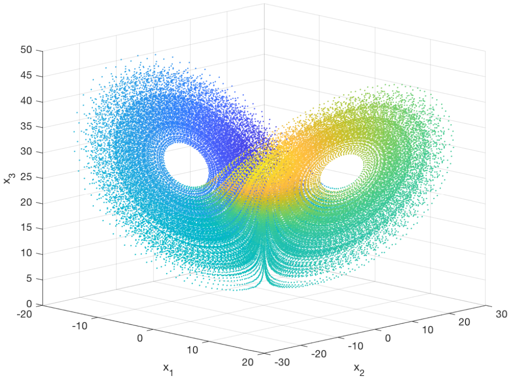
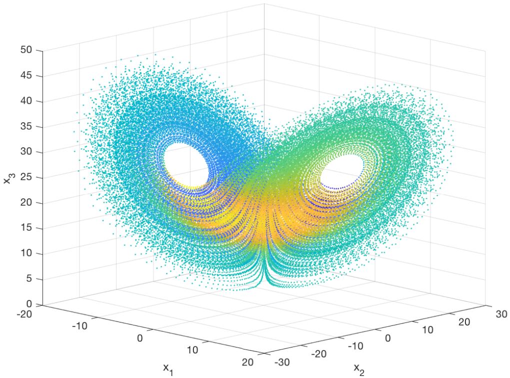


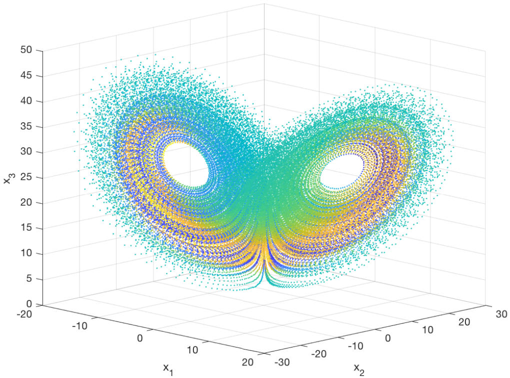

$$f(x) = x_1, \quad x = (x_1, x_2, x_3)$$



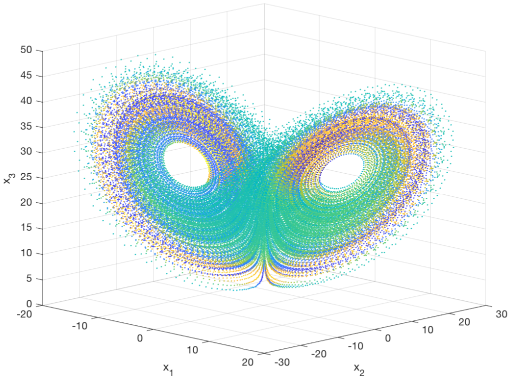

$$f(\Phi^t(x)), \quad t = 0.2$$



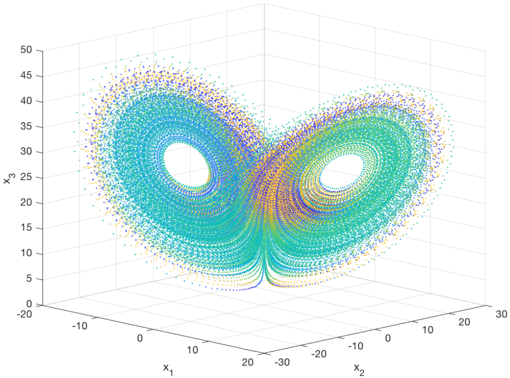

$$f(\Phi^t(x)), \quad t = 0.4$$



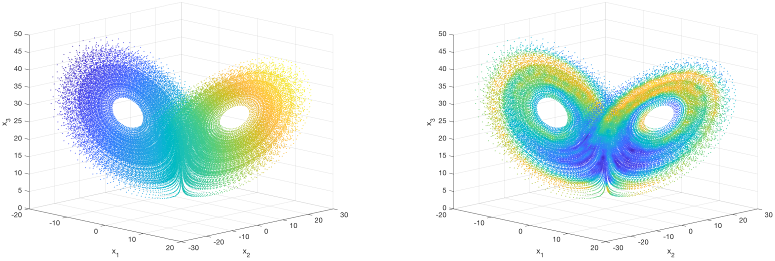

$$f(\Phi^t(x)), \quad t = 0.6$$



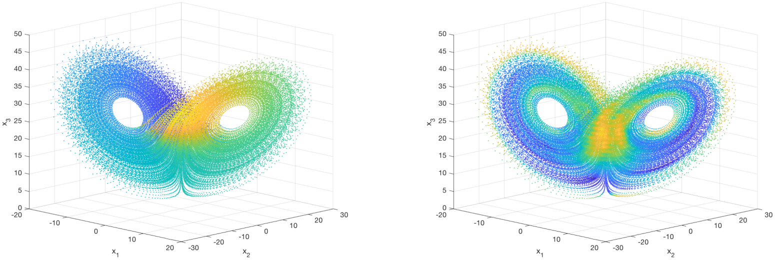

$$f(\Phi^t(x)), \quad t = 0.8$$



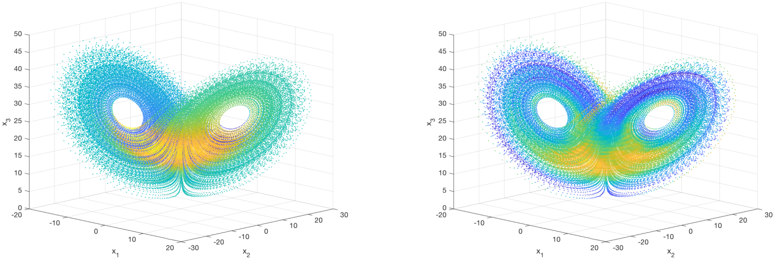

$$f(\Phi^t(x)), \quad t = 1$$




$t = 0$




$t = 0.2$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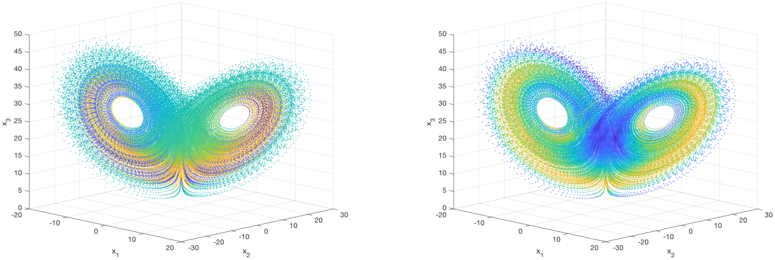
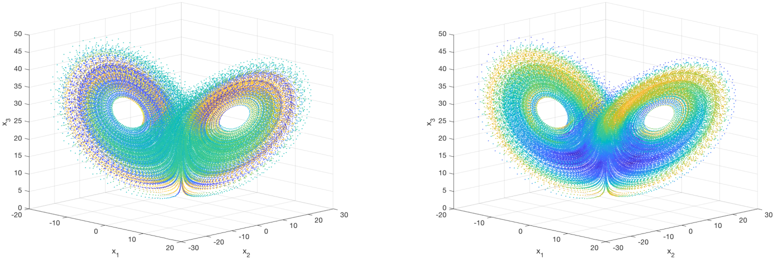
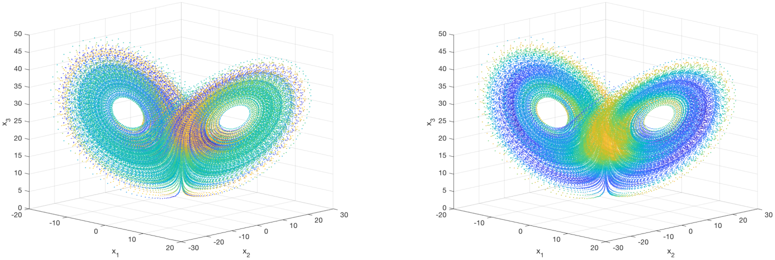
$t = 0.4$



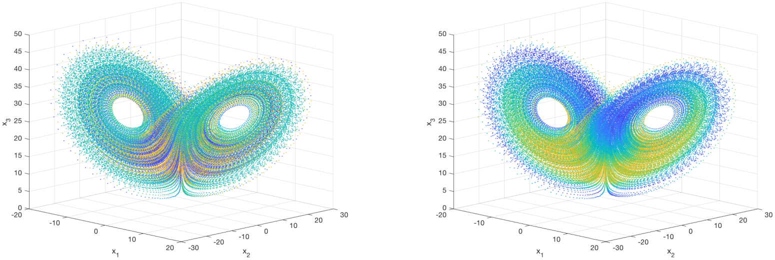

$$t = 0.6$$



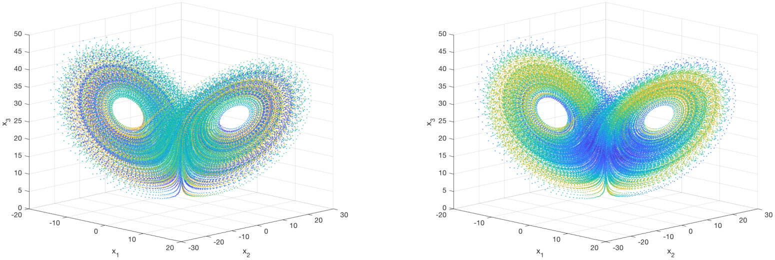

$$t = 0.8$$



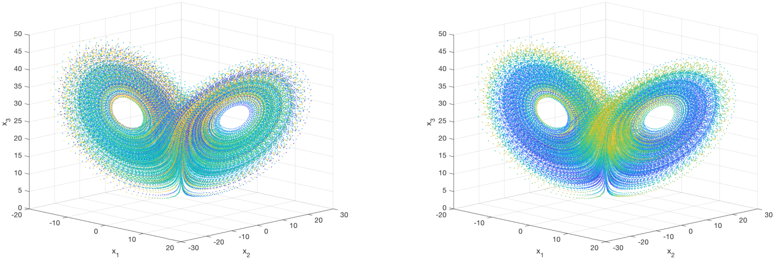

$$t = 1$$



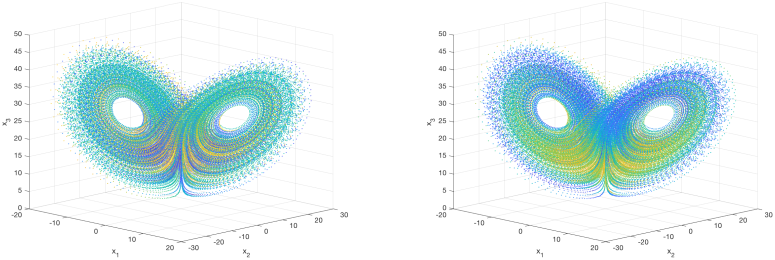

$t = 2$



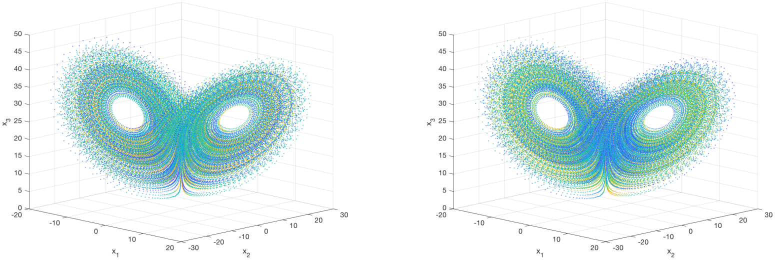

$t = 3$



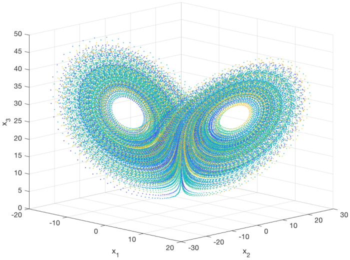

$t = 4$




$t = 5$




$t = 15$



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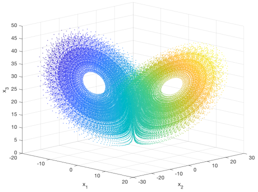
$t = 20$

## Setup and basic assumptions




- Continuous flow $\Phi^t : \mathcal{M} \to \mathcal{M}$, $t \in \mathbb{R}$, on metric space $\mathcal{M}$
- Ergodic, invariant Borel probability measure $\mu$ with compact support $X \subseteq \mathcal{M}$
- Forward-invariant, compact, $C^1$ manifold $M \subseteq \mathcal{M}$, s.t. $X \subseteq M$ and $\Phi^t|_M$ is $C^1$

- Koopman operators $U^t : f \mapsto f \circ \Phi^t$ on $C^0(M)$, $L^2(\mu)$
- Generator $V : D(V) \to L^2(\mu)$,

$$D(V) \subset L^2(\mu), \quad V^* = -V, \quad Vf = \lim_{t \to 0} (U^t f - f)/t$$

- Projection-valued measure $E : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mu))$,

$$V = \int_{\mathbb{R}} i\omega \, dE(\omega), \quad U^t = \int_{\mathbb{R}} e^{i\omega t} \, dE(\omega)$$

## Objectives

1. Identify **coherent observables** under the dynamics
*(spectral approximation of operators)*

2. Perform **forecasting** of observables
*(pointwise approximation of operators)*

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

- Many operator theoretic techniques developed to address these objectives (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; Williams et al. 2015; Klus et al. 2016; Brunton et al. 2017; G. 2017; Das & G. 2017; Wu & Noé 2017; Korda et al. 2018; . . . )
- Here, discuss approaches to address these objectives using ideas from **reproducing kernel Hilbert space (RKHS) theory** (Das et al. 2018)

| | $C^0(M)$ | $L^2(\mu)$ | RKHS $\mathcal{H}$ |
|---|---|---|---|
| Pointwise evaluation | ✓ | × | ✓ |
| Inner product | × | ✓ | ✓ |
| Dynamics-intrinsic | ✓ | ✓ | × |

## Reproducing kernel Hilbert spaces

An RKHS $\mathcal{H}$ on $M$ is a Hilbert space of functions $f : M \to \mathbb{C}$ such that, for every $x \in M$, the **evaluation functional** $J_x : f \mapsto f(x)$ is bounded

Every RKHS $\mathcal{H}$ has a unique **reproducing kernel**, $k : M \times M \to \mathbb{C}$ s.t.

1. $k(x, \cdot) \in \mathcal{H}$, $\forall x \in M$
2. $k(x, y) = k(y, x)^*$, $\forall x, y \in M$
3. For every $x_0, \ldots, x_{n-1} \in M$, the $n \times n$ kernel matrix $\boldsymbol{K} = [k(x_i, x_j)]$ is positive-semidefinite
4. For every $x \in M$ and $f \in \mathcal{H}$, $f(x) = J_x f = \langle k(x, \cdot), f \rangle_{\mathcal{H}}$

Conversely, for every $k : M \times M \to \mathbb{C}$ satisfying the above properties, there exists a unique RKHS $\mathcal{H}$ with $k$ as its reproducing kernel (Moore-Aronszajn thm.)

If $k \in C^r(M \times M)$, then $\mathcal{H} \subset C^r(M)$, and the inclusion $\mathcal{H} \hookrightarrow \mathbb{C}^r$ is bounded (Ferreira & Menegatto 2013)

## RKHS and integral operators

Let $\nu$ be a finite Borel measure on $M$ with compact support $X_\nu \subseteq M$, and $\mathcal{H}$ an RKHS with continuous reproducing kernel $k$

- The following **integral operator** $K : L^2(\nu) \to \mathcal{H}$ is well-defined:

$$K : f \mapsto \int_M k(\cdot, x) f(x) \, d\nu(x)$$

- $K^*$ coincides with the inclusion map $C^0(M) \hookrightarrow L^2(\nu)$
- $G = K^* K$ is a self-adjoint, positive-semidefinite, trace-class integral operator on $L^2(\nu)$

- There exists an orthonormal basis $\{\phi_0, \phi_1, \dots\}$ of $L^2(\nu)$ consisting of eigenfunctions of $G$ at real eigenvalues $\lambda_0 \geq \lambda_1 \geq \cdots \searrow 0$
- $\psi_j = K\phi_j / \lambda_j^{1/2}$, $\lambda_j > 0$, forms an orthonormal basis of $\overline{\operatorname{ran} K} \subseteq \mathcal{H}$
- $k(x, y) = \sum_j \psi_j(x) \psi_j(y)$, uniformly for $x, y \in X_\nu$ (Mercer thm.)

- $k$ is said to be **$L^2(\nu)$-strictly-positive** if $G > 0$
- $k$ is said to be **$L^2(\nu)$-Markov ergodic** if (i) $Gf = f$ iff. $f = \text{const}$; (ii) $Gf \geq 0$ if $f \geq 0$; (iii) $\langle 1, Gf \rangle_\mu = \langle 1, f \rangle_\mu$

## Nyström extension

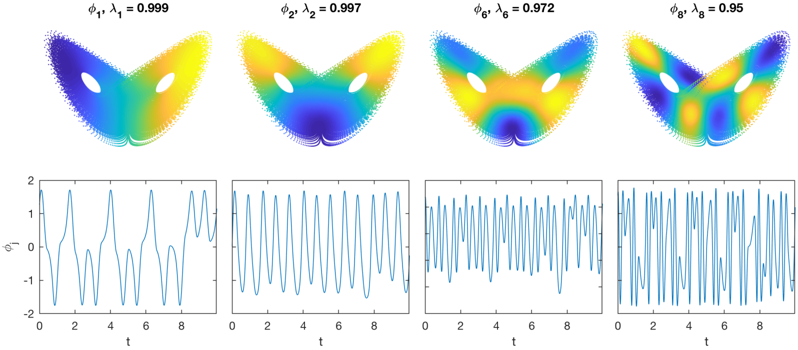
Let $H = \operatorname{ran} K^* \subseteq L^2(\nu)$, and define $\mathcal{N} : H \to \mathcal{H}$ s.t.

$$\mathcal{N} : \sum_j c_j \phi_j \mapsto \sum_j \lambda_j^{-1/2} c_j \psi_j$$

- $\mathcal{N} f$ is an **extension** of $f$ in the sense that $K^* \mathcal{N} f = f$
- $\operatorname{ran} \mathcal{N} = \overline{\operatorname{ran} K}$, and $\mathcal{N}^\dagger = K^*$
- $H$ acquires Hilbert space structure via the inner product $\langle f, g \rangle_H = \langle \mathcal{N} f, \mathcal{N} g \rangle_{\mathcal{H}}$; $H \hookrightarrow L^2(\nu)$ then becomes a compact embedding
- If $k$ is $L^2(\nu)$-strictly-positive, $H$ is a dense subspace of $L^2(\nu)$
- If $k$ is $L^2(\nu)$-Markov ergodic, $\|f\|_H \geq \|f\|_{L^2(\nu)}$, with equality iff $f = \text{const}$.
- The associated **Dirichlet energy** $\mathcal{D} : H \to \mathbb{R}_+$ then assigns a measure of **roughness** of functions in $H$,

$$\mathcal{D}(f) = \frac{\|f\|_H^2}{\|f\|_{L^2(\nu)}^2} - 1$$

# Eigenfunctions of $G_N$ on the L63 attractor



## RKHS compactification schemes for the generator

Because $V$ is a skew-adjoint extension of the dynamical vector field $\vec{V} : C^1(M) \to L^2(\mu)$, given an RKHS $\mathcal{H}$ with $C^1$ reproducing kernel $k$,

$$\operatorname{ran} G = \operatorname{ran} K^* K \subseteq \operatorname{ran} K^* \subset D(V)$$

**Pre-smoothing:**

- $A = VG$ is a Hilbert-Schmidt integral operator on $L^2(\mu)$ with $C^0$ kernel $k'(\cdot, x) = \vec{V} k(\cdot, x)$, i.e.,

$$Af = \int_M k'(\cdot, x) f(x)\, d\mu(x)$$

**Post-smoothing:**

- $GV : D(V) \to L^2(\mu)$ is a densely-defined bounded operator, whose closure, $\overline{GV} = (GV)^{**} =: B$ is equal to $-A^*$, i.e.,

$$GV \subset -A^* = B, \quad Bf = -\int_M k'(x, \cdot) f(x)\, d\mu(x)$$

## RKHS compactification schemes for the generator

### Skew-adjoint compactification on $\mathcal{H}$:

- $W = KVK^*$ is a skew-adjoint, Hilbert-Schmidt operator on $\mathcal{H}$ given by

$$Wf = -\int_M k'(x,\cdot) f(x)\, d\mu(x)$$

- The operator $K^* W \mathcal{N} : H \to L^2(\mu)$ is a restriction of $B$

### Skew-adjoint compactification on $L^2(\mu)$:

- $G^{1/2} V G^{1/2}$ is a densely-defined, bounded, antisymmetric operator, whose closure is a skew-adjoint, Hilbert-Schmidt operator $\tilde{V} : L^2(\mu) \to L^2(\mu)$
- There is a partial isometry $\mathcal{U} : L^2(\mu) \to \mathcal{H}$, given by the polar decomposition $K = \mathcal{U} G^{1/2}$, s.t. $\tilde{V} = \mathcal{U}^* W \mathcal{U}$

## Spectra of the compactified generators

Let $k$ be $L^2(\mu)$-strictly-positive, Markov ergodic, and define $\mathcal{K} = \overline{\operatorname{ran} K} \subseteq \mathcal{H}$

- $A$, $B$, $\tilde{V}$, and $W|_{\mathcal{K}}$ have the same, purely imaginary, spectra, including multiplicities of eigenvalues
- There exist orthonormal bases $\{\tilde{z}_0, \tilde{z}_1, \dots\}$ and $\{\zeta_0, \zeta_1, \dots\}$ of $L^2(\mu)$ and $\mathcal{K}$, respectively, s.t.,

$$\tilde{V}\tilde{z}_j = i\omega_j z_j, \quad W\zeta_j = i\omega_j\zeta_j, \quad \omega_j \in \mathbb{R}, \quad \zeta_j = \mathcal{U} z_j$$

- 0 is a simple eigenvalue of $A$, $B$, $\tilde{V}$, and $W|_{\mathcal{K}}$ corresponding to constant eigenfunctions
- $z_j' = G^{-1/2}\tilde{z}_j$ and $z_j = G^{1/2}\tilde{z}_j$ are eigenfunctions of $A$ and $B$, respectively, and $\{z_0', z_1', \dots\}$ and $\{z_0, z_1, \dots\}$ form biorthogonal, unconditional Schauder bases of $L^2(\mu)$
- The following expansions converge in operator norm:

$$W = \sum_{j=0}^{\infty} i\omega_j \langle \zeta_j, \cdot \rangle_{\mathcal{H}} \zeta_j, \quad \tilde{V} = \sum_{j=0}^{\infty} i\omega_j \langle \tilde{z}_j, \cdot \rangle_{L^2(\mu)} \tilde{z}_j$$

- The following expansions converge strongly:

$$A = \sum_{j=0}^{\infty} i\omega_j \langle z_j, \cdot \rangle_{L^2(\mu)} z_j', \quad B = \sum_{j=0}^{\infty} i\omega_j \langle z_j', \cdot \rangle_{L^2(\mu)} z_j$$

## Functional calculus

- Associated with $\tilde{V}$ and $W$ are unique, purely-atomic **projection-valued measures (PVMs)** $E : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(L^2(\mu))$ and $\mathcal{E} : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$, s.t.

$$\tilde{E}(\Omega) = \sum_{j:\omega_j \in \Omega} \langle \tilde{z}_j, \cdot \rangle_{L^2(\mu)} \tilde{z}_j, \quad \mathcal{E}(\Omega) = \sum_{j:\omega_j \in \Omega} \langle \zeta_j, \cdot \rangle_{\mathcal{H}} \zeta_j + 1_\Omega(0) \operatorname{proj}_{\mathcal{K}^\perp}$$

$$\tilde{E}(\Omega) = \mathcal{U}^* \mathcal{E}(\Omega) \mathcal{U}$$

$$\tilde{V} = \int_{\mathbb{R}} i\omega \, d\tilde{E}(\omega), \quad W = \int_{\mathbb{R}} i\omega \, d\mathcal{E}(\omega)$$

- Given a Borel-measurable function $Z : i\mathbb{R} \to \mathbb{C}$, we compute

$$Z(\tilde{V}) = \int_{\mathbb{R}} Z(i\omega) \, d\tilde{E}(\omega) = \sum_{j=0}^{\infty} Z(i\omega_j) \langle \tilde{z}_j, \cdot \rangle_{L^2(\mu)} \tilde{z}_j,$$

$$Z(W) = \int_{\mathbb{R}} Z(i\omega) \, d\mathcal{E}(\omega) = \sum_{j=0}^{\infty} Z(i\omega_j) \langle \zeta_j, \cdot \rangle_{\mathcal{H}} \zeta_j + Z(0) \operatorname{proj}_{\mathcal{K}^\perp}$$

- Being non-normal, $A$ and $B$ generally do not have associated PVMs, but it is still possible to define an associated **holomorphic functional calculus**

## Spectral convergence

Let $\{k_\tau\}_{\tau>0}$ be a one-parameter family of $C^1$, $L^2(\mu)$-strictly-positive kernels s.t., as $\tau \to 0^+$,

1. $G_\tau = K_\tau^* K_\tau \to I$, pointwise on $L^2(\mu)$
2. $\tilde{V}_\tau \to V$, pointwise on $D(V^2) \subset D(V)$

$D(V^2)$ is a **core** for $V$, and as a result condition 2 implies that $\tilde{V}_\tau$ converges to $V$ in **strong resolvent sense**

The latter, in conjunction with compactness and skew-adjointness of the approximating operators $\tilde{V}_\tau$ implies in turn the following:

- As $\tau \to 0^+$, $B_\tau$ converges strongly to $V$ on $D(V)$
- For every bounded, continuous function $Z : i\mathbb{R} \to \mathbb{C}$, as $\tau \to 0^+$, $Z(\tilde{V}_\tau)$ and $K_\tau^* Z(W_\tau)\mathcal{N}_\tau$ converge strongly to $Z(V)$
- For every bounded Borel-measurable set $\Omega \subset \mathbb{R}$ such that $E(\partial\Omega) = 0$, as $\tau \to 0^+$, $\tilde{E}_\tau(\Omega)$ and $K_\tau^* \mathcal{E}_\tau(\Omega)\mathcal{N}_\tau$ converge strongly to $E(\Omega)$
- For every element of the spectrum $i\omega$ of $V$, there exists a sequence of eigenvalues $i\omega_\tau$ of $\tilde{V}_\tau$ (and $A_\tau$, $B_\tau$, $W_\tau$) converging to $i\omega$ as $\tau \to 0^+$

## Markov semigroups

To construct a one-parameter family of kernels meeting the previously stated conditions:

1. Start from a $C^1$, $L^2(\mu)$-strictly positive, Markov ergodic kernel $p : M \times M \to \mathbb{R}$, constructed, e.g., by normalization of an unnormalized kernel (Coifman & Hirn 2013)
2. Compute the eigenvalues and eigenfunctions of the associated operator $G = P^* P : L^2(\mu) \to L^2(\mu)$, i.e., $G\phi_j = \lambda_j \phi_j$, and $1 = \lambda_0 > \lambda_1 \geq \lambda_2 \geq \cdots > 0$
3. For every $\tau > 0$ and $x, y \in M$, define

$$p_\tau(x,y) = \sum_{j=0}^{\infty} \frac{e^{-\tau \eta_j}}{\lambda_j} \psi_j(x)\psi_j(y), \quad \eta_j = \frac{1}{\lambda_j} - 1, \quad \psi_j = \frac{1}{\lambda_j^{1/2}} P\phi_j$$

Then, the following hold:

- The series for $p_\tau(x,y)$ converges to a $C^1$ reproducing kernel $p_\tau$ of an RKHS $\mathcal{H}_\tau \subset \mathcal{H}$ in $C^1(M \times M)$ norm
- $\mathcal{H}_\tau$ has an orthonormal basis with elements $\psi_{\tau,j} = e^{-\tau\eta_j/2} P_\tau \phi_j$, and $\mathcal{H}_{\tau_1} \subseteq \mathcal{H}_{\tau_2}$ whenever $\tau_1 \geq \tau_2$
- Defining $G_0 = I$ and $G_\tau = P_\tau^* P_\tau$, the family $\{G_\tau\}_{\tau \geq 0}$ is a strongly continuous, self-adjoint, Markov semigroup
- As $\tau \to 0^+$, the corresponding approximate generator $\tilde{V}_\tau$ is **of trace class**, and converges to $V$, pointwise on $D(V)$, as required

## Coherent pattern extraction

- Given $t \in \mathbb{R}$ and $\epsilon > 0$, a complex number $\gamma$ is said to lie in the **$\epsilon$-approximate point spectrum of $U^t$** if there exists a nonzero $f \in L^2(\mu)$ such that

$$\|U^t f - \gamma f\|_{L^2(\mu)} < \epsilon \|f\|_{L^2(\mu)}$$

- Define $R : \mathbb{R}_+ \times \mathbb{R}_+ \to \mathbb{R}$,

$$R(\epsilon, \tau) := \sup\{T > 0 : \|(U^t - e^{tB_\tau})P^*\| < \epsilon,\ \forall t \in [-T, T]\}$$

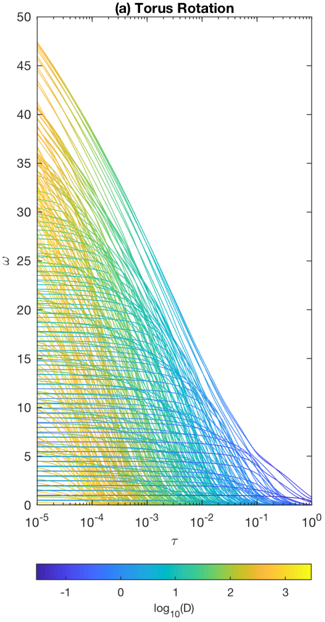
Let $(i\omega_\tau, \zeta_\tau)$ be an eigenpair of $W_\tau$. Then, $(e^{i\omega_\tau t}, \tilde{z}_\tau)$, with $\tilde{z}_\tau = P_\tau^* \zeta_\tau$, is an $\epsilon$-approximate eigenpair of $U^t$ for all $t \in (-\mathcal{T}(\epsilon, \tau), \mathcal{T}(\epsilon, \tau))$, where

$$\mathcal{T}(\epsilon, \tau) = R(\epsilon, \tau)/\sqrt{\mathcal{D}(\tilde{z}_\tau) + 1}.$$

In addition:

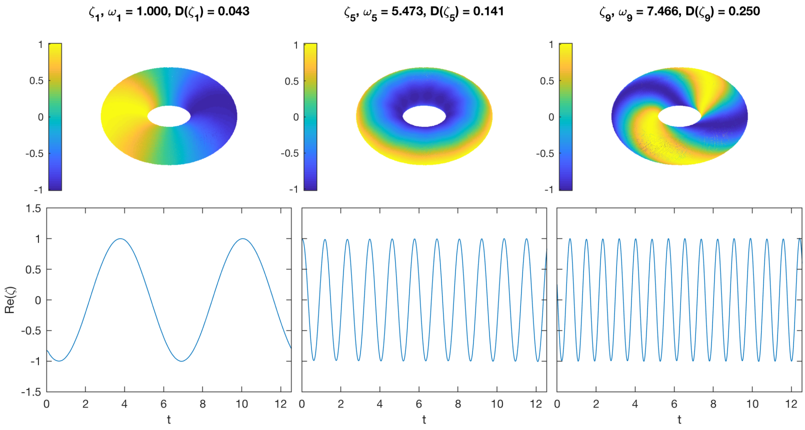
1. If $\lim_{\tau \to 0^+} \omega_\tau =: \omega$ exists, and $\mathcal{T}(\epsilon, \tau)$ diverges as $\tau \to 0^+$ for every $\epsilon > 0$, then $i\omega$ is an element of the spectrum of $V$.
2. If $\lim_{\tau \to 0^+} \omega_\tau =: \omega$ exists, and $\mathcal{D}(\tilde{z}_\tau)$ is bounded as $\tau \to 0^+$, then $i\omega$ is an eigenvalue of $V$. Moreover, the sequence $\tilde{z}_\tau$ converges to the eigenspace of $V$ corresponding to $i\omega$.

# Torus rotation—spectra of $W_\tau$




- $\mathcal{M} = M = X = \mathbb{T}^2$
- $\Phi^t : (\theta^1, \theta^2) \mapsto (\theta^1 + t, \theta^2 + \alpha t)$
- $\alpha = \sqrt{30}$

# Torus rotation—eigenfunctions of $W_\tau$



## Data-driven modeling scenario

Consider that a **time-ordered dataset** $F(x_0), \dots, F(x_{N-1})$, $x_n = \Phi^{n\,\Delta t}(x_0)$, is available, s.t.

- $F : M \to Y$ is a $C^1$, injective map into a manifold $Y$
- $\mu$ is an ergodic invariant measure of $\Phi^{\Delta t}$
- $x_0$ lies in the **basin** of $\mu$; i.e., as $N \to \infty$, the sampling measures $\mu_N$ weak-converge to $\mu$:

$$\lim_{N\to\infty} \int_M f \, d\mu_N = \int_M f \, d\mu, \quad \forall f \in C^0(M), \quad \mu_N = \frac{1}{N} \sum_{n=0}^{N-1} \delta_{x_n}$$

- $x_0$ is not a fixed point

## Approximating the kernel integral operators

- Replace $L^2(\mu)$ by $L^2(\mu_N)$
- Construct a $L^2(\mu_N)$-strictly positive, $C^1$, Markov ergodic kernel $p_N : M \times M \to \mathbb{R}$ as a **pullback kernel** from the data space $Y$:

$$p_N(x, y) = \rho_N(F(x), F(y))$$

- Let $\mathcal{H}_N$ be the RKHS on $M$ associated with $p_N$; define $P_N : L^2(\mu_N) \to \mathcal{H}_N$ and $\mathcal{H}_{N,\tau}$ as in the case of $\mu$

- Under mild assumptions, as $N \to \infty$, $p_N \to p$ in $C^0(M \times M)$ (G. et al. 2017), and the corresponding kernel integral operators on $C^0(M)$ converge **collectively compactly** (Von Luxburg et al. 2008)
- As a result, for every eigenvalue $\lambda_j > 0$ of $G = P^* P$, $\lambda_{j,N}$ converges to $\lambda_j$, where $\lambda_{j,N}$ are eigenvalues of $G_N = P_N^* P_N$
- For every eigenfunction $\phi_j \in L^2(\mu)$ corresponding to $\lambda_j > 0$, there exist eigenfunctions $\phi_{j,N} \in L^2(\mu_N)$ of $G_N = P_N^* P_N$ corresponding to $\lambda_{j,N}$ whose continuous representatives, $\varphi_{j,N}$, converge in $C^0(M)$ to the continuous representative $\varphi_j$ of $\phi_j$:

$$\varphi_{j,N}(x) = \frac{1}{\lambda_{j,N}} \int_M p_N(x, y) \phi_{j,N}(y) \, d\mu_N(y), \quad \varphi_j(x) = \frac{1}{\lambda_j} \int_M p(x, y) \phi_j(y) \, d\mu(y)$$

## Approximating the evolution operators

- Replace the Koopman operator $U^t : f \mapsto f \circ \Phi^t$ on $L^2(\mu)$ at $t = q\,\Delta t$, $q \in \mathbb{N}_0$, by the **shift operator** $U_N^{(q)} : L^2(\mu_N) \to L^2(\mu_N)$,

$$U_N^{(q)} f(x_n) = \begin{cases} f(x_{n+q}), & 0 \le n \le N-1-q, \\ 0, & \text{otherwise} \end{cases}$$

- Replace the generator $V$ by a **skew-adjoint, finite-difference operator** $V_{N,\Delta t} : L^2(\mu_N) \to L^2(\mu_N)$, e.g.,

$$V_{N,\Delta t} = \frac{\tilde{V}_{N,\Delta t} - \tilde{V}^*_{N,\Delta t}}{2}, \quad \tilde{V}_{N,\Delta t} f(x_n) = \begin{cases} \frac{f(x_n) - f(x_n - 1)}{\Delta t}, & 1 \le n \le N-1, \\ 0, & \text{otherwise} \end{cases}$$

- Introduce the orthogonal projections $\Pi_{\tau,N,L} : \mathcal{H}_{\tau,N} \to \mathcal{H}_{\tau,N}$ mapping into $\operatorname{span}\{\psi_{0,\tau,N}, \dots, \psi_{L-1,\tau,N}\}$
- Replace $W_\tau : \mathcal{H}_\tau \to \mathcal{H}_\tau$ by the skew-adjoint operator $W_{\tau,N,\Delta t,L}$ on $\mathcal{H}_{\tau,N}$,

$$W_{\tau,N,\Delta t,L} = \Pi_{\tau,N,L} P^*_{\tau,N} V_{N,\Delta t} P_{\tau,N} \Pi_{\tau,N,L}$$

- Solve the eigenproblem for $W_{\tau,N,\Delta t,L}$:

$$W_{\tau,N,\Delta t,L} \zeta_j^{(\tau,N,\Delta t,L)} = i\omega_j^{(\tau,N,\Delta t,L)} \zeta_j^{(\tau,N,\Delta t,L)}$$

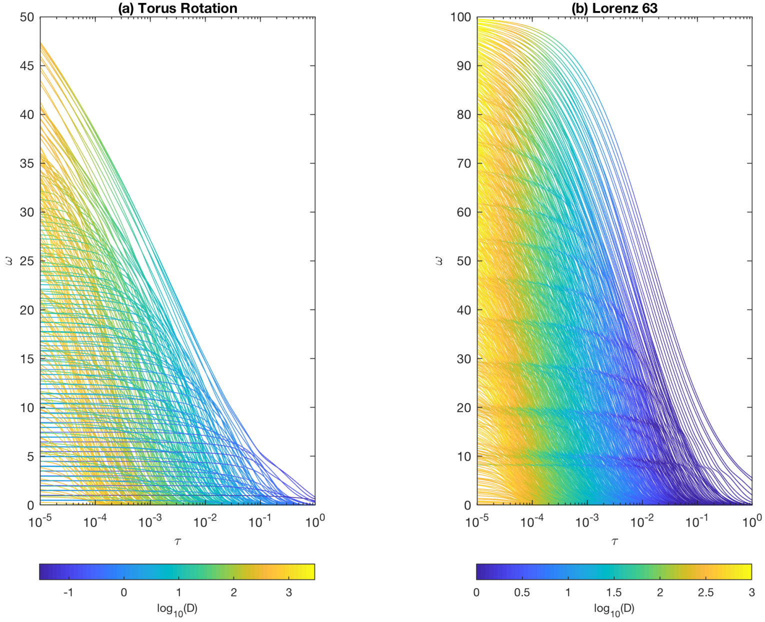
- Functional calculus for $W_{\tau,N,\Delta t,L}$ constructed analogously to $W_\tau$

## Convergence of the data-driven schemes

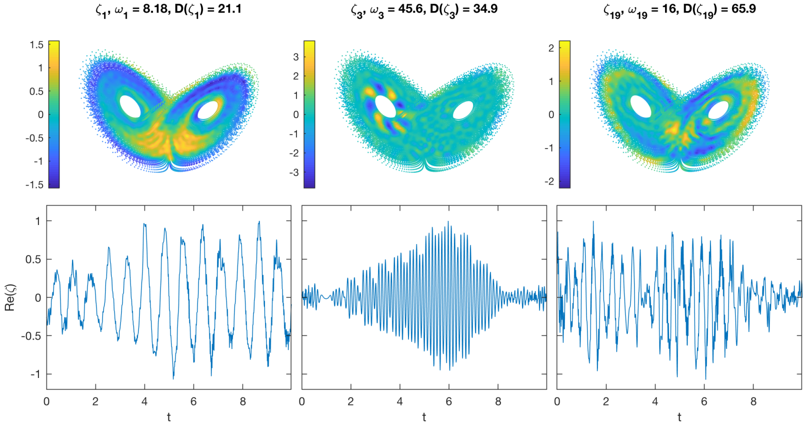
- Introduce the orthogonal projections $\Pi_{\tau,L} : \mathcal{H}_\tau \to \mathcal{H}_\tau$ mapping into $\operatorname{span}\{\psi_{0,\tau}, \dots, \psi_{L-1,\tau}\}$, and define the finite-rank operator $W_{\tau,L} = \Pi_{L,\tau} W_\tau \Pi_{L,\tau}$
- At fixed $L$ and as $\Delta t \to 0$, $N \to \infty$ (in that order), the eigenvalues $i\omega_j^{(\tau,N,\Delta t,L)}$ converge to the eigenvalues $i\omega_j^{(\tau,L)}$ of $W_{\tau,L}$, and the corresponding eigenfunctions converge in $C^0(M)$ norm
- At fixed $\tau$ and as $L \to \infty$, the eigenvalues $i\omega_j^{(\tau,L)}$ converge to the eigenvalues $i\omega_j^{(\tau)}$ of $W_\tau$, and the corresponding eigenfunctions converge in $\mathcal{H}_\tau$ norm
- For every $i\omega \in \sigma(V)$, there exists a continuous curve of eigenvalues of $W_\tau$ converging to it as $\tau \to 0^+$; moreover, for every bounded Borel-measurable set $\Omega \subset \mathbb{R}$ such that $E(\partial\Omega) = 0$, $P_\tau^* \mathcal{E}_\tau(\Omega) \mathcal{N}_\tau$ converges strongly to $E(\Omega)$

- In summary, **spectral convergence** of $W_{\tau,N,\Delta t,L}$ to $V$ is to be understood in a joint limit of $N \to \infty$, $\Delta t \to 0$, $L \to \infty$, $\tau \to 0^+$ (in that order)

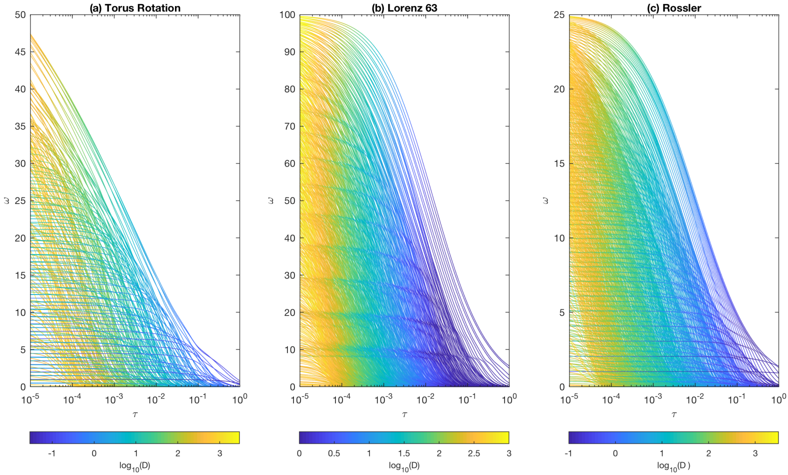
# Lorenz 63 system—spectra of $W_\tau$



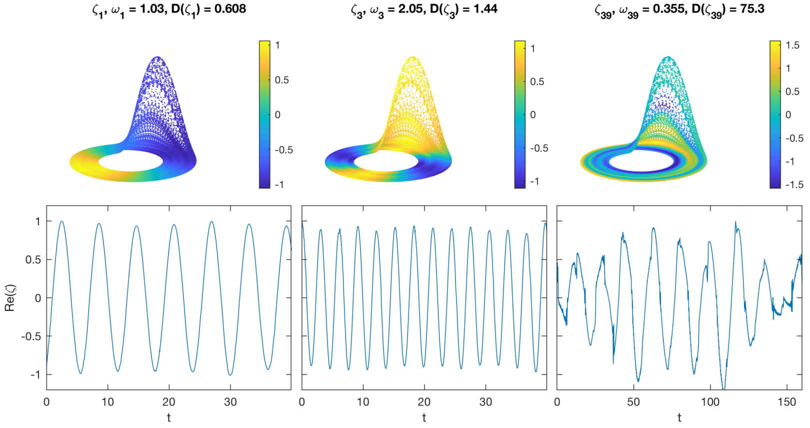
# L63 system—eigenfunctions of $W_\tau$



# Rössler system—spectra of $W_\tau$



# Rössler system—eigenfunctions of $W_\tau$

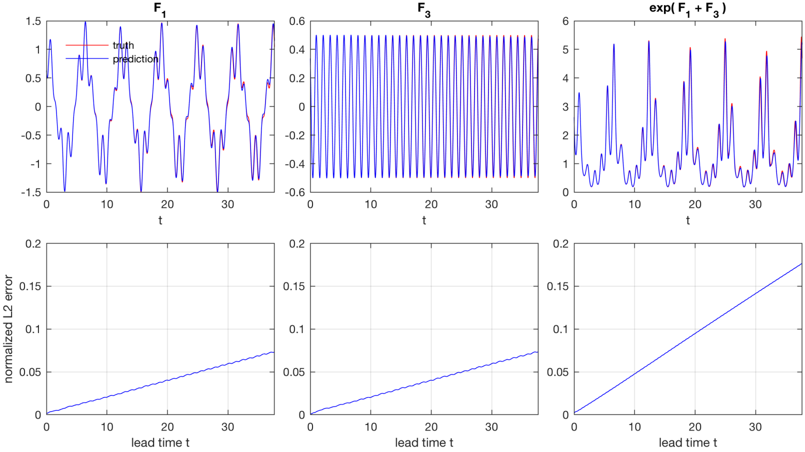


## Prediction of observables

- For every $\tau > 0$, $W_\tau$ generates a **norm-continuous** group of unitary operators $e^{tW_\tau} : \mathcal{H}_\tau \to \mathcal{H}_\tau$, $t \in \mathbb{R}$, approximating $U^t$
- For any observable $f \in L^2(\mu)$, error bound $\epsilon > 0$, and compact set $\mathcal{T} \subset \mathbb{R}$, there exists $\hat{f}_\epsilon \in \cap_{\tau>0}\mathcal{H}_\tau$ (independent of $\mathcal{T}$) and $\tau_0 > 0$, such that for every $\tau \in (0, \tau_0)$ and $t \in \mathcal{T}$,

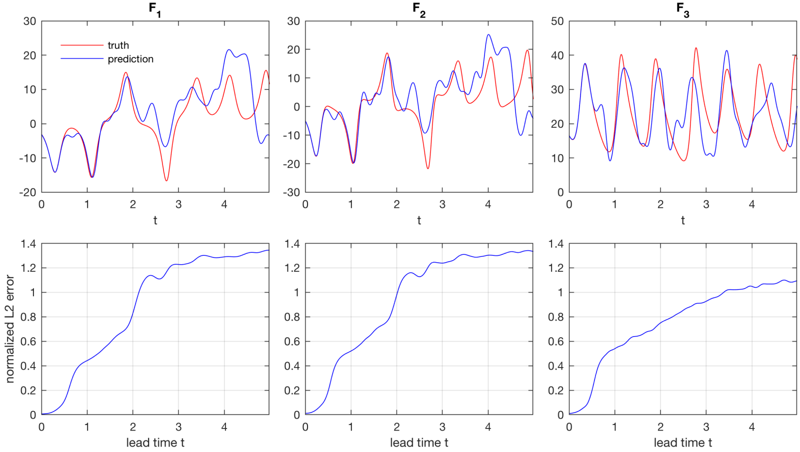
$$\left\| U^t f - P_\tau^* e^{tW_\tau} f_\epsilon \right\|_{L^2(\mu)} < \epsilon, \quad e^{tW_\tau} f_\epsilon = \sum_{j=0}^{\infty} e^{ti\omega_{\tau,j}} \langle \zeta_{\tau,j}, f_\epsilon \rangle_{\mathcal{H}_\tau} \zeta_{\tau,j}$$

## Torus rotation—prediction of observables using $e^{tW_\tau}$



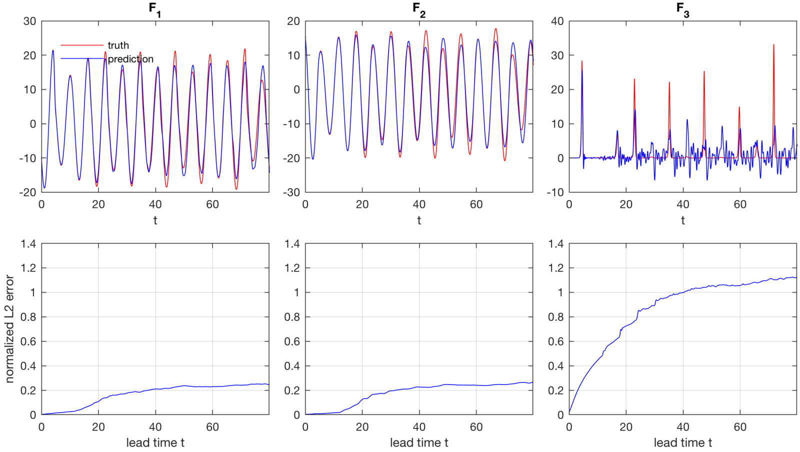

$$F : \mathbb{T}^2 \to \mathbb{R}^3, \quad (\theta_1, \theta_2) \mapsto \begin{pmatrix} (1 + R\cos\theta_2)\cos\theta_1 \\ (1 + R\cos\theta_2)\sin\theta_1 \\ \sin\theta_2 \end{pmatrix}$$

# L63 system—prediction of observables using $e^{tW_\tau}$




$$F : \mathbb{R}^3 \to \mathbb{R}^3, \quad F = I$$

# Rössler system—prediction of observables using $e^{tW_\tau}$

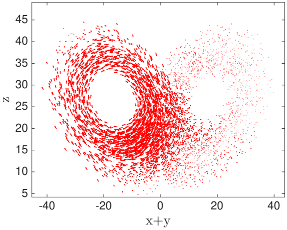



$$F : \mathbb{R}^3 \to \mathbb{R}^3, \quad F = I$$

## Conclusions

- Kernel methods provide a useful framework for data-driven prediction and spectral decomposition in ergodic dynamical systems
- Advantages of the approach include the ability to construct bases for function spaces of appropriate regularity with minimal prior knowledge about the system
- Regularization approach based on compactification of the generator in a space of functions of high regularity (RKHS), as opposed to adding diffusion, leads to a notion of coherent observables in systems with continuous spectra and an approximation framework for the functional calculus of the generator

### Ongoing and future work:




- Data assimilation and control
- Spectral approximation of vector fields and differential forms (exterior calculus)
  (Berry & G. 2018)
- Applications to climate and fluid dynamics

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