Section 4

Spectral theory

Setting and objectives

General assumptions

- $\Phi : G \times \Omega \to \Omega$: Continuous-time, continuous flow on compact, metrisable space Ω.
- μ: Ergodic invariant Borel probability measure.
- $X : \Omega \to \cancel{\mathbb{X}}$ continuous observation map into metric space $\mathcal{X}$.
- $U^t : \mathcal{F} \to \mathcal{F}$: Koopman operator on Banach space $\mathcal{F}$ of complex-valued observables.

$C(\Omega)$
$L^p(\mu)$

Given. Time-ordered samples

$$x_n = X(\omega_n), \quad \omega_n = \Phi^{t_n}(\omega_0), \quad t_n = (n-1)\,\Delta t.$$

Feature extraction

Goal. Using the data x_n, identify a collection of observables $\zeta_j : \Omega \to \mathcal{Y}$ which have the property of evolving coherently under the dynamics in a suitable sense.

Setting and objectives

We recall the following facts from Section 2 (Theorems 2.29 and2.30).

Theorem 4.1. Under our general assumptions:

C_0 groups (or semigroups)

1. *The evolution group* $\{U^t : C(\Omega) \to C(\Omega)\}_{t\in\mathbb{R}}$ *is* $\boxed{\textit{strongly continuous}}$*.*
2. *The evolution group* $\{U^t : L^p(\mu) \to L^p(\mu)\}_{t\in\mathbb{R}}$*,* $p \in [\cancel{0}1, \infty)$ *is strongly continuous.*
3. *The evolution group* $\{U^t : L^\infty(\mu) \to L^\infty(\mu)\}_{t\in\mathbb{R}}$ *is* ~~*weakly*~~ weak-* *continuous.*

$\{U^t\}$ is a group under composition of operators:

- $U^s \circ U^t = U^{s+t}$
- $U^0 = Id$
- $(U^t)^{-1} = U^{-t}$

For every $f \in L^\infty(\mu)$ and $g \in L^1(\mu)$,

$$\lim_{t\to 0} \int g\, U^t f \, d\mu = \int g f \, d\mu$$

For every $f \in C(\Omega)$

$$\lim_{t\to 0} U^t f = f \text{ in } C(\Omega) \text{ norm}$$

$\Updownarrow$

$t \longmapsto U^t f$ is continuous at 0

$\Downarrow$ + group property

$t \longmapsto U^t f$ is continuous at every $t \in \mathbb{R}$.

KOOPMAN EIGENFUNCTIONS IN $C(\Omega)$

$$U^t z = \Lambda_t z, \qquad \begin{array}{l} z \in C(\Omega)\setminus\{0\}, \text{ Koopman eigenfunction} \\ \Lambda_t \in \mathbb{C}, \text{ Koopman eigenvalue} \end{array}$$

Recall: U^t acts as a $*$-isomorphism of $C(\Omega)$, viewed as a C^*-algebra of functions, i.e., $\forall f, g \in C(\Omega)$,

(1) $$U^t(fg) = (U^t f)(U^t g), \quad (U^t f)^* = U^t f^*, \quad \|U^t f\|_{C(\Omega)} = \|f\|_{C(\Omega)}$$

Suppose z, z' are Koopman eigenfunctions corresponding to eigenvalues Λ_t, Λ_t'.

Then, using (1),

$$U^t(zz') = (U^t z)(U^t z') = (\Lambda_t z)(\Lambda_t' z') = \Lambda_t \Lambda_t' (zz')$$

$\Rightarrow$ zz' is also an eigenfunction, corresponding to $\Lambda_t \Lambda_t'$.

Moreover,

$$U^t(z^*) = (U^t z)^* = (\Lambda_t z)^* = \Lambda_t^* z^*$$

$\Rightarrow$ z^* is an eigenfunction corresponding to Λ_t^*.

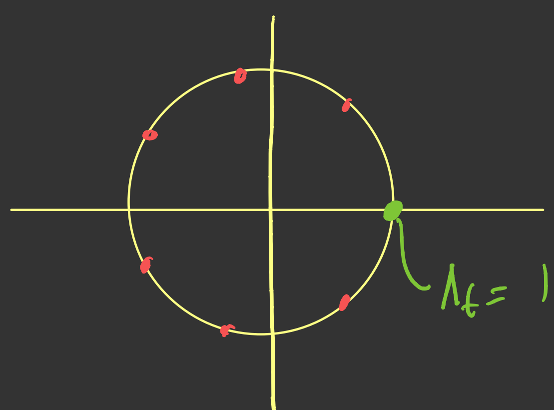
Moreover,

$$U^t|z|^2 = U^t(z^* z) = (U^t z^*)(U^t z) = \Lambda_t^* z^* \Lambda_t z = \underbrace{|\Lambda_t|^2}_{=1} |z|^2$$

And since U^t is an isometry,

$$\|z\|_{C(\Omega)} = \|U^t z\|_{C(\Omega)} = \|\Lambda_t z\|_{C(\Omega)} = |\Lambda_t| \, \|z\|_{C(\Omega)} \Rightarrow |\Lambda_t| = 1$$

$\Rightarrow$ The eigenvalues of U^t lie on the unit circle in $\mathbb{C}$.



Using the previously established properties we deduce that the set of eigenvalues of U^t forms a multiplicative subgroup S^1.

point spectrum $= \sigma_p(U^t; C(\Omega))$

- $\Lambda_t, \Lambda_t' \in \sigma_p(U^t; C(\Omega)) \Rightarrow \Lambda_t \Lambda_t' \in \sigma_p(U^t; C(\Omega))$ (closed under $\circ$)
- $1 \in \sigma_p(U^t; C(\Omega))$ (identity element)
- $\Lambda_t^{-1} = \Lambda_t^*$ (inverse)

similarly, the normalized eigenfunctions form a multiplicative semigroup / group

By the group property of U^t, if $U^t z = \Lambda_t z$ we have

$$U^{s+t} z = U^s \circ U^t z = U^s \Lambda_t z = \Lambda_t U^s z$$

$\Rightarrow$ $U^s z$ is also an eigenfunction at eigenvalue Λ_t

<u>Claim:</u> Suppose that $\phi^t : \Omega \to \Omega$ is measure-preserving and ergodic. Then if $z \in C(\Omega)$ is a continuous eigenfunction of U^t, there exists $\alpha \in \mathbb{R}$ s.t. $\Lambda_t = e^{i\alpha t}$. Moreover, z can be normalized s.t. $|z| = 1$.

$$\Rightarrow U^t z = e^{i\alpha t} z \quad \Rightarrow z \text{ has a periodic evolution under } U^t$$

with period $2\pi/\alpha$.

Let $R_t^\alpha : S^1 \to S^1$ be the circle rotation with frequency α. Then, the following diagram commutes:

$$\begin{tikzcd}
\Omega \arrow[r, "\phi^t"] \arrow[d, "z"'] & \Omega \arrow[d, "z"] \\
S^1 \arrow[r, "R_t^\alpha"] & S^1
\end{tikzcd}$$

topological semi-conjugacy to a circle rotation

Setting and objectives

We recall the following facts from Section 2 (see Proposition 2.7 and Theorems 2.29, 2.30).

Theorem 4.1.

1. $\{U^t : C(\Omega) \to C(\Omega)\}_{t\in\mathbb{R}}$ *is a strongly continuous group of isometries.*
2. $\{U^t : L^p(\mu) \to L^p(\mu)\}_{t\in\mathbb{R}}$, $p \in [0, \infty)$ *is a strongly continuous group of isometries. Moreover,* $U^t : L^2(\mu) \to L^2(\mu)$ *is unitary.*
3. $\{U^t : L^\infty(\mu) \to L^\infty(\mu)\}_{t\in\mathbb{R}}$ *is a weak-* continuous group of isometries.*

Notation.

- $\mathcal{F}$: Any of the $C(\Omega)$ or $L^p(\mu)$ spaces with $1 \leq p \leq \infty$.
- $\mathcal{F}_0$: Any of the $C(\Omega)$ or $L^p(\mu)$ spaces with $1 \leq p < \infty$.
- C_0 (semi)group $\equiv$ strongly continuous (semi)group.
- C_0^* (semi)group $\equiv$ weak-* continuous (semi)group.

Generator of C_0 semigroups

Definition 4.2.
Let $\{S^t\}_{t\geq 0}$ be a C_0 semigroup on a Banach space E. The generator $A : D(A) \to E$ of the semigroup $\{S^t\}_{t\geq 0}$ is defined as

$$Af = \lim_{t\to 0} \frac{S^t f - f}{t}, \quad f \in D(A),$$

where the limit is taken in the norm of E, and the domain $D(A) \subseteq E$ consists of all $f \in E$ for which the limit exists.

Example 1 (circle rotation)

$\phi^t : S^1 \to S^1$ $\phi^t(\omega) = \omega + \alpha t \mod 2\pi$. Consider $U^t : C(\Omega) \to C(\Omega)$.

For every $f \in C^1(\Omega)$, $\omega \in S^1$,

$$\lim_{t\to 0} \frac{U^t f(\omega) - f(\omega)}{t} = \lim_{t\to 0} \frac{f(\phi^t(\omega)) - f(\omega)}{t} = \lim_{t\to 0} \alpha \frac{f(\omega+\alpha t) - f(\omega)}{\alpha t} = f'(\omega)\alpha$$

Moreover the convergence to the limit is uniform wrt $\omega \in S^1$, i.e.,

$$\lim_{t\to 0} \left\| \frac{U^t f - f}{t} - \alpha f' \right\|_{C(\Omega)} = \lim_{t\to 0} \max_{\omega\in S^1} \left| \frac{f(\omega+\alpha t) - f(\omega)}{t} - \alpha f'(\omega) \right| = 0$$

$\Rightarrow D(A) \supseteq C^1(\Omega)$. In fact, in this case $D(A) = C^1(\Omega)$

Moreover the operator A is <u>unbounded</u>.

First, we say that $A : D(A) \to E$ is bounded if $\displaystyle\sup_{f \in E \setminus \{0\}} \frac{\|Af\|_E}{\|f\|_E} < \infty$

A is said to be <u>unbounded</u> if no such bound exists.

For our example, $A : D(\Omega) \to C(\Omega)$ is unbounded because we have a sequence $f_n(\omega) = e^{in\omega}$, $n \in \mathbb{N}$ such that

$$\frac{\|Af_n\|_{C(\Omega)}}{\|f_n\|_{C(\Omega)}} = \frac{\|\alpha f_n'\|_{C(\Omega)}}{\|f_n\|_{C(\Omega)}} = \frac{\|\alpha i n f_n\|_{C(\Omega)}}{\|f_n\|_{C(\Omega)}} = |\alpha| n.$$

That is, f_n is a sequence of unit vectors in $C(\Omega)$, for which $\|Af_n\|_{C(\Omega)}$ increases without bound.

<u>Example 2</u> With Φ^t as above, consider $U^t : L^2(\mu) \to L^2(\mu)$. Here,

$$Af = \lim_{t \to 0} \frac{U^t f - f}{t}.$$

in L^2 norm

In this case, $C^1(\Omega)$ is a strict subspace of $D(A)$.

In fact, $D(A) = H^1(\mu)$

Sobolev space of order 1

= Elements of L^2 that have L^2 derivatives.

Generator of C_0 semigroups

D(A) is a dense subspace of E
$\Leftrightarrow$ $\forall f \in E$ and $\varepsilon > 0$ there exists $g \in D(A)$
s.t. $\|f-g\|_E < \varepsilon$.
e.g. $C^1(S^1)$ is a dense subspace of $C(S^1)$.

Theorem 4.3.
With the notation of Definition 4.2, the following hold.

1. *A is closed and densely defined.*
2. *For all $f \in D(A)$ and $t \geq 0$, the function $t \mapsto S^t f$ is continuously differentiable, and satisfies*

$$\frac{d}{dt} S^t f = AS^t f = S^t Af.$$

3. *A uniquely characterizes the semigroup $\{S^t\}$, i.e., if $\{\tilde{S}^t\}$ is another C_0 semigroup on E with the same generator A, then $S^t = \tilde{S}^t$ for all $t \geq 0$.*

A is closed if
for every $f_n \in D(A)$ that converges to $f \in E$
such that $g_n = Af_n$ also converges to $g \in E$,
then we have (i) $f \in D(A)$
(ii) $g = Af$

Generator of C_0^* semigroups

e.g., $L^\infty(\mu)$ e.g. $L^1(\mu)$

Definition 4.4.
Let $\{S^t\}_{t\geq 0}$ be a C_0^* semigroup on a Banach space E with predual E_*.
The generator $A : D(A) \to E$ of the semigroup $\{S^t\}_{t\geq 0}$ is defined as the weak-* limit

$$\langle g, Af \rangle = \lim_{t\to 0} \frac{\langle g, S^t f - f\rangle}{t}, \quad f \in D(A), \quad \forall g \in E_*,$$

where the domain $D(A) \subseteq E$ consists of all $f \in E$ for which the limit exists.

e.g. for $g \in L^1(\mu)$, $f \in L^\infty(\mu)$

$\langle g, Af \rangle = \int_\Omega g \, Af \, d\mu$

Theorem 4.5.

With the notation of Definition 4.4, the following hold.

1. *A is weak-* closed and densely defined.*
2. *For all $f \in D(A)$ and $t \geq 0$, the function $t \mapsto S^t f$ is weak-* continuously differentiable, and satisfies*

$$\left\langle g, \frac{d}{dt} S^t f \right\rangle = \langle g, AS^t f\rangle = \langle g, S^t Af\rangle.$$

3. *A uniquely characterizes the semigroup $\{S^t\}$, i.e., if $\{\tilde{S}^t\}$ is another C_0^* semigroup on E with the same generator A, then $S^t = \tilde{S}^t$ for all $t \geq 0$.*

Generator of unitary C_0 groups

$S^{t*} = S^{-t}$

Theorem 4.6 (Stone).
Let $\{S^t\}_{t\geq 0}$ be a unitary C_0 group on a Hilbert space H. Then, the generator $A : D(A) \to H$ is skew-adjoint, i.e.,

$$A^* = -A.$$

Conversely, if $A : D(A) \to H$ is skew-adjoint, it is the generator of a unitary evolution group.

If A is skew-adjoint, it is antisymmetric i.e., for every $f, g \in D(A)$, $\langle f, Ag\rangle_H = -\langle Af, g\rangle_H$

In finite-dimensional spaces, antisymmetric $\equiv$ skew-adjoint.

In infinite dimensions, not every antisymmetric operator is skew-adjoint.

Example: $\Phi^t : S^1 \to S^1$ circle rotation, $U^t : L^2(\mu) \to L^2(\mu)$.

Can define $\tilde{A} : D(\tilde{A}) \to L^2(\mu)$ as a densely defined operator with domain $D(\tilde{A}) = C^1(S^1)$ as $\tilde{A}f = \lim_{t\to 0} \frac{U^t f - f}{t}$. Then, it follows by integration parts that $\tilde{A}$ is antisymmetric. However, it is not skew-adjoint. In contrast, the generator $A : D(A) \to L^2(\mu)$ with $D(A) = H^1(\mu)$ is skew-adjoint.

We can think of A as a <u>skew-adjoint extension</u> of $\tilde{A}$ i.e.,

$$\tilde{A}f = Af \quad \text{for } f \in D(\tilde{A}) = C^1(\Omega), \quad \text{but} \quad \underset{\substack{\| \\ H^1(\Omega)}}{D(A)} \supset D(\tilde{A}).$$

Generator of Koopman evolution groups

$\mathcal{F}_0$ stands for either $C(\Omega)$ or $L^p(\mu)$ for $1 \le p < \infty$.

Corollary 4.7.

Under our general assumptions the following hold:

1. *The Koopman evolution groups $U^t : \mathcal{F}_0 \to \mathcal{F}_0$ are uniquely characterized by their generator $V : D(V) \to \mathcal{F}_0$, where*

$$Vf = \lim_{t \to 0} \frac{U^t f - f}{t}.$$

Moreover, for $\mathcal{F}_0 = L^2(\mu)$, V is skew-adjoint.

2. *The Koopman evolution group $U^t : L^\infty(\mu) \to L^\infty(\mu)$ is uniquely characterized by its generator $V : D(V) \to \mathcal{F}_0$, where*

$$Vf = \lim_{t \to 0} \frac{U^t f - f}{t}$$

in weak-* sense.

Generator of Koopman evolution groups

Theorem 4.8 (ter Elst & Lemańczyk).
Let (Ω, Σ) be a compact metrisable space equipped with its Borel σ-algebra Σ. Let μ be a Borel probability measure on Ω and $U^t : L^2(\mu) \to L^2(\mu)$ a C_0 unitary evolution group with generator $V : D(V) \to L^2(\mu)$. Then, the following are equivalent.

1. *For every $t \in \mathbb{R}$ there exists a μ-a.e. invertible, measurable, and measure-preserving flow $\Phi^t : \Omega \to \Omega$ such that $U^t f = f \circ \Phi^t$.*
2. *The space $\mathfrak{A}(V) = D(V) \cap L^\infty(\mu)$ is an algebra with respect to function multiplication, and V is a derivation on $\mathfrak{A}$:*

$$V(fg) = (Vf)g + f(Vg), \quad \forall f, g \in \mathfrak{A}(V).$$

Leibniz rule

$\Delta \phi_j = \lambda_j \phi_j$

for $f = \sum_j c_j \phi_j$

Counter example Δ: (self-adjoint) Laplacian on a Reimannian manifold,

$U^t f = e^{it\Delta} f = \sum_j c_j e^{i\lambda_j t} \phi_j$

$U^t = e^{it\Delta}$ is a C_0 unitary group on L^2

but it is not realized by a flow ϕ^t since Δ does not satisfy the Leibniz rule

Point spectrum

Definition 4.9.
Let $A : D(A) \to E$ be an operator on a Banach space with domain $D(A) \subseteq E$. The point spectrum of A, denoted as $\sigma_p(A) \subseteq \mathbb{C}$ is defined as the set of its eigenvalues. That is, $\lambda \in \mathbb{C}$ is an element of $\sigma_p(A)$ iff there is a nonzero vector $u \in E$ (an eigenvector) such that

$$Au = \lambda u.$$

Notation.

- We use the notation $\sigma_p(A; E)$ when we wish to make explicit the Banach space on which A acts.

Eigenvalues and eigenfunctions

Definition 4.10.
Let $A : D(A) \to E$ be the generator of a C_0 semigroup $\{S^t\}_{t \geq 0}$ on a Banach space E. We say that $\lambda \in \mathbb{C}$ is an eigenvalue of the semigroup if λ is an eigenvalue of A, i.e., there exists a nonzero $u \in D(A)$ such that

$$Au = \lambda u.$$

Lemma 4.11.
With notation as above, λ is an eigenvalue of $\{S^t\}$ if and only if z is an eigenvector of S^t for all $t \geq 0$, i.e., there exist $\Lambda^t \in \mathbb{C}$ such that

$$S^t u = \Lambda^t u, \quad \forall t \geq 0.$$

In particular, we have $\Lambda^t = e^{\lambda t}$.

Pf. Suppose $S^t u = \Lambda^t u$. We show that $Au = \lambda u$ where $\Lambda^t = e^{\lambda t}$.

Since S^t is a C_0 semigroup, $t \longmapsto S^t u = \Lambda^t u$ is a continuous function satisfying

(i) $\Lambda^0 = 1$ (since $S^0 = Id$)

(ii) $\Lambda^{s+t} = \Lambda^s \Lambda^t$ (since $S^{s+t} = S^s S^t$).

The only function with these properties is the exponential function, $\Lambda^t = e^{\lambda t}$ for some $\lambda \in \mathbb{C}$. We have

$$Au = \lim_{t \to 0} \frac{S^t u - u}{t} = \lim_{t \to 0} \frac{\Lambda^t u - u}{t} = \left(\lim_{t \to 0} \frac{e^{\lambda t} - 1}{t} \right) u = \frac{d}{dt} e^{\lambda t} \Big|_{t=0} u = \lambda u \quad \checkmark$$

Now suppose $Au = \lambda u$. We show that $S^t u = \Lambda^t u$ for $\Lambda^t = e^{\lambda t}$.

Since $u \in D(A)$ we have that $S^t u$ is the unique solution of the equation

$$\frac{d}{dt} S^t u = AS^t u = S^t A u = \lambda S^t u. \quad (*)$$

It follows by substitution that $S^t = e^{\lambda t} u$ satisfies $(*)$. Since, as can be shown, solutions to $(*)$ are unique, the claim follows. $\checkmark$

$\square$

Return to the Koopman operators $U^t : L^p(\mu) \longrightarrow L^p(\mu)$

Previously, we saw that because U^t acts on $L^p(\mu)$ by isometries, every eigenvalue Λ^t of U^t lies on the unit circle.

$$U^t f = \Lambda^t f \implies \|U^t f\|_{L^p(\mu)} = |\Lambda^t| \, \|f\|_{L^p(\mu)} \implies |\Lambda^t| = 1.$$

As a result every eigenvalue λ of the generator is purely imaginary.
i.e. if $\Lambda^t = e^{\lambda t} \in S^1$ then $\lambda = i\alpha$ for some $\alpha \in \mathbb{R}$.

Conclusion: Every eigenfunction u of U^t is a periodic observable, i.e.,

$$U^t u = \Lambda^t u = e^{\lambda t} u = e^{i\alpha t} u$$

with period $2\pi/\alpha$.

This motivates using Koopman eigenfunctions as coherent observables of the system.

Point spectra for measure-preserving flows

Theorem 4.12.
Let $\Phi^t : \Omega \to \Omega$ a be a measure-preserving flow of a probability space (Ω, Σ, μ). Let $U^t : L^p(\mu) \to L^p(\mu)$ be the associated Koopman operators on $L^p(\mu)$, $p \in [1, \infty]$, and $V : D(V) \to L^p(\mu)$ the corresponding generators. Then, the following hold.

1. *For every $p, q \in [1, \infty]$ and $t \in \mathbb{R}$, $\sigma_p(U^t, L^p(\mu)) = \sigma_p(U^t, L^q(\mu))$.*
2. *$\sigma_p(V, L^p(\mu)) = \sigma_p(V, L^q(\mu))$.* Recall $L^p(\mu) \subset L^q(\mu)$ when $p > q$
3. *$\sigma_p(U^t)$ is a subgroup of S^1.*
4. *$\sigma_p(V)$ is a subgroup of $i\mathbb{R}$.*

Idea of proof: For any $\lambda \in \mathbb{C}$ $\ker U^t - \lambda \big|_{L^\infty(\mu)}$ is a dense subspace of $\ker U^t - \lambda \big|_{L^p(\mu)}$.

Corollary 4.13.
Every eigenfunction of V lies in $L^\infty(\mu)$, and thus in $L^p(\mu)$ for every $p \in [1, \infty]$.

Given $\lambda = i\alpha \in \sigma_p(V)$, we say that α is an eigenfrequency of V.

Group structure of $\sigma_p(U^t)$ and $\sigma_p(V)$

Suppose $u_1, u_2 \in L^\infty(\mu)$ are eigenfunctions of U^t at eigenvalues Λ_1^t, Λ_2^t. Then

$$U^t(u_1u_2) = (U^t u_1)(U^t u_2) = \Lambda_1^t \Lambda_2^t u_1 u_2 \Rightarrow \Lambda_1^t\Lambda_2^t \in \sigma_p(U^t)$$

$\Rightarrow \sigma_p(U^t)$ is closed under multiplication

Moreover, $U^t \bar{u}_1 = \overline{(U^t u_1)} = \overline{\Lambda_1^t}\, \bar{u}_1 \Rightarrow \overline{\Lambda_1^t} \in \sigma_p(U^t) \Rightarrow \sigma_p(U^t)$ closed under complex conj.

Moreover, since $|\Lambda_1^t|^2 = \overline{\Lambda_1^t}\Lambda_1 = 1 \Rightarrow \overline{\Lambda_1^t} = 1/\Lambda_1^t \Rightarrow \sigma_p(U^t)$ has a multiplicative inverse

Also, we have $U^t 1 = 1 \Rightarrow \Lambda^t = 1 \in \sigma_p(U^t)$

We conclude that $\sigma_p(U^t)$ is a countable subgroup of S^1.

Now since $\Lambda^t = e^{\lambda t}$ it follows that $\sigma_p(V)$ is an (additive) subgroup of $i\mathbb{R}$

i.e. if $\lambda_1, \lambda_2 \in \sigma_p(V)$ $\lambda_1 + \lambda_2$ is also an eigenvalue, etc.

Generating frequencies

Definition 4.14.
Assume the notation of Theorem 4.12.

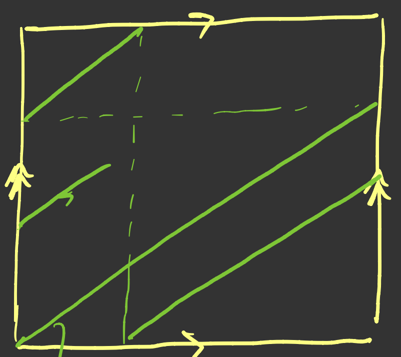
1. We say that $\{ia_0, ia_1, \ldots\} \subseteq \sigma_p(V)$ is a generating set if for every $i\alpha \in \sigma_p(V)$ there exist $j_1, j_2, \ldots, j_n \in \mathbb{Z}$ and $k_1, k_2, \ldots, k_n \in \mathbb{N}$ such that
$$\alpha = j_1 \alpha_{k_1} + j_2 \alpha_{k_2} + \ldots + j_n \alpha_{k_n}.$$
2. We say that $\sigma_p(V)$ is finitely generated if it has a finite generating set.
3. A generating set is said to be minimal if it does does not have any proper subsets which are generating sets.

Lemma 4.15.

1. *The elements of a minimal generating set are rationally independent.*
2. *If a minimal generating set has at least two elements, then $\sigma_p(V)$ is a dense subset of the imaginary line.*

Example: Ergodic rotation on $\mathbb{T}^2$.

$$\Phi^t(\omega_1,\omega_2) = (\omega_1+\alpha_1 t, \omega_2+\alpha_2 t) \bmod 2\pi, \quad \alpha_1,\alpha_2 \in \mathbb{R}, \text{ rationally indep.}$$



For $f \in C^1(\mathbb{T}^2)$,

$$Vf(\omega_1,\omega_2) = \lim_{t\to 0} \frac{U^t f(\omega_1,\omega_2) - f(\omega_1,\omega_2)}{t} = \alpha_1 \frac{\partial f}{\partial \omega_1}(\omega_1,\omega_2) + \alpha_2 \frac{\partial f}{\partial \omega_2}(\omega_1+\omega_2)$$

For $j=(j_1,j_2) \in \mathbb{Z}^2$

Consider the Fourier functions $\phi_j(\omega_1,\omega_2) = e^{i(j_1\omega_1 + j_2\omega_2)}$

$$V\phi_j = \alpha_1 \frac{\partial}{\partial \omega_1}\phi_j + \alpha_2 \frac{\partial}{\partial \omega_2}\phi_j = \underbrace{i(j_1\alpha_1 + j_2\alpha_2)}_{\text{Eigenfrequency } \alpha_j}\phi_j$$

Since $\{\phi_j\}_{j\in\mathbb{Z}}$ forms an orthonormal basis of $L^2(\mu)$, we have identified a
normalized Lebesgue
complete set of linearly independent eigenfunctions, and we conclude

$$\sigma_p(V) = \{i\alpha_j\}_{j\in\mathbb{Z}^2}$$

dense subset of $i\mathbb{R}$.

$\{i\alpha_1, i\alpha_2\}$ is a minimal generating set.

Generating frequencies

Lemma 4.16.
Let $g_1, g_2, \ldots$ be eigenfunctions corresponding to the eigenvalues of the generating set in Definition 4.14, i.e., $Vg_j = i\alpha_j g_j$. Then, for every $i\alpha \in \sigma_p(V)$ with $\alpha = j_1\alpha_{k_1} + j_2\alpha_{k_2} + \ldots + j_n\alpha_{k_n}$,

$$z = g_{k_1}^{j_1} g_{k_2}^{j_2} \cdots g_{k_n}^{j_n}$$

is an eigenfunction of V corresponding to the eigenfrequency α.

Invariant subspaces

Notation.

- $H_p = \overline{\operatorname{span}\{u \in L^2(\mu) \colon u \text{ is an eigenfunction of } V\}}$.
- $H_c = H_p^\perp$. "continuous spectrum subspace"
- $\{z_0, z_1, \dots\}$: Orthonormal eigenbasis of H_p, $Vz_j = i\alpha_j z_j$.

Theorem 4.17.
Let $\Phi^t : \Omega \to \Omega$ be a measure-preserving flow on a completely metrizable space with an invariant probability measure μ.

1. *H_p and H_c are U^t-invariant subspaces.*
2. *Every $f \in H_p$ satisfies*

$$U^t f = \sum_{j=0}^{\infty} \hat{f}_j e^{i\alpha_j t} z_j, \quad \hat{f}_j = \langle z_j, f \rangle_{L^2(\mu)}.$$

Observables in H_c have "weak mixing" behavior.

3. *Every $f \in H_c$ satisfies*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |\langle g, U^t f \rangle_{L^2(\mu)}| \, dt = 0, \quad \forall g \in L^2(\mu).$$

Pure point spectrum

Definition 4.18.
With the notation of Theorem 4.17, we say that a measure-preserving flow $\Phi^t : \Omega \to \Omega$ has pure point spectrum if $H_p = L^2(\mu)$.

$\Leftrightarrow$ V is unitarily diagonalizable

Remark 4.19.
For a system with pure point spectrum:

1. The spectrum of V is not necessarily discrete. as long as there are ≥ 2 generating frequencies $\sigma_p(V)$ is a dense subset of $i\mathbb{R}$
2. The continuous spectrum is not necessarily empty.

The spectrum of V contains $\overline{\sigma_p(V)}$
Elements in $\overline{\sigma_p(V)} \setminus \sigma_p(V)$ lie in the continuous spectrum of V.

Point spectra for ergodic flows

$\Rightarrow f \in L^p(\mu)$, $U^t f = f$ for all t
$f = \text{const.}$ μ-a.e.

Proposition 4.20.

With the notation of Theorem 4.12, assume that $\Phi^t : \Omega \to \Omega$ is ergodic.

1. *Every eigenvalue $\lambda \in \sigma_p(V)$ is simple.*
2. *Every corresponding eigenfunction $z \in L^p(\mu)$ normalized such that $\|z\|_{L^p(\mu)} = 1$ for any $p \in [1, \infty]$ satisfies $\underbrace{|z| = 1}_{\text{unimodular}}$ μ-a.e.*

Suppose that $U^t z = \Lambda^t z$ for all $t \in \mathbb{R}$ with $\Lambda^t = e^{\lambda t}$. Then,

$U^t |z|^2 = U^t(\bar{z} z) = (U^t \bar{z})(U^t z) = \overline{\Lambda^t} \Lambda^t |z|^2 = |z|^2$

By ergodicity, $|z|^2 = \text{const.}$ μ-a.e. and can be normalized such that $|z| = 1$ μ-a.e.

$\Rightarrow$ Suppose that w is another eigenfunction corresponding to Λ^t, i.e. $U^t w = \Lambda^t w$. We have,

$U^t(\bar{w} z) = \overline{\Lambda^t} \Lambda^t \bar{w} z = \bar{w} z \Rightarrow \bar{w} z$ is constant μ-a.e. $\Rightarrow w$ is a multiple of z

$\Rightarrow \lambda$ is simple.

Factor maps

Definition 4.21.
Let $T_1 : \Omega_1 \to \Omega_1$ and $T_2 : \Omega_2 \to \Omega_2$ be measure-preserving transformations of the probability spaces $(\Omega_1, \Sigma_1, \mu_1)$ and $(\Omega_2, \Sigma_2, \mu_2)$. We say that T_2 is a factor of T_1 if there exists a T_1-invariant set $S_1 \in \Sigma_1$ with $\mu_2(S_{\cancel{1}})$ 2 $= 1$, a T_2-invariant set $S_2 \in \Sigma_2$ with $\mu_2(S_2) = 1$, and a measure-preserving, surjective map $\varphi : S_1 \to S_2$ such that

$$T_2 \circ \varphi = \varphi \circ T_1.$$

Such a map φ is called a factor map and satisfies the following commutative diagram:

$$\begin{tikzcd} S\cancel{M}_1 \arrow[r, "T_1"] \arrow[d, "\varphi"'] & \cancel{M}_1 S \arrow[d, "\varphi"] \\ S\cancel{M}_2 \arrow[r, "T_2"] & S\cancel{M}_2 \end{tikzcd}.$$

<u>Prop.</u> Let $\phi^t : \Omega \to \Omega$ be an ergodic measure-preserving flow of a standard probability space (Ω, Σ, μ). Let $i\alpha \in \sigma_p(V)$, $R^t : S^1 \to S^1$ $R^t(\theta) = \theta + \alpha t \bmod 2\pi$. Let $Vz = i\alpha z$, normalized s.t. $|z| = 1$. Then $R^t \circ z = z \circ \phi^t$ is a factor map.

Example Variable-frequency rotation.

Let $\phi^t : S^1 \longrightarrow S^1$ be the solution map of the ODE

$$\dot{\omega}(t) = \beta(\omega(t))$$

for $\beta : S^1 \longrightarrow \mathbb{R}$ a strictly positive continuous function.

In this case, the generator V, applied to a C^1 function f, is given by

$$Vf = \beta f'$$

Consider the eigenvalue problem

$$Vz(\omega) = \lambda z(\omega) \iff \beta(\omega)\frac{dz}{d\omega} = \lambda z(\omega) \quad (*)$$

period/2π $\parallel$

Change of variables $d\theta = \frac{C}{\beta(\omega)}\, d\omega$ i.e. $\theta(\omega) = C\int_0^{\omega} \frac{1}{\beta(\omega')}\, d\omega'$ where C is such that $\theta(\omega) = 2\pi$

Then $(*)$ becomes $\frac{dz(\omega(\theta))}{d\theta} = \frac{1}{C}\lambda z(\theta(\omega)) \Rightarrow \lambda = \frac{1}{C} ij$ for $j \in \mathbb{Z}$

and $z(\theta(\omega)) = e^{ij\theta(\omega)}$

"modified Fourier function"

On the basis of the proposition the following diagram should commute:

$$\begin{tikzcd} S^1 \arrow[r, "\phi^t"] \arrow[d, "z"'] & S^1 \arrow[d] \\ S^1 \arrow[r, "R^t"] & S^1 \end{tikzcd}$$

where R^t is circle rotation with frequency $1/C$.

Metric isomorphisms

Definition 4.22.
With the notation of Definition 4.21, we say that T_1 and T_2 are measure-theoretically isomorphic or metrically isomorphic if there is a factor $\varphi : S_1 \to S_2$ with a measurable inverse.

Theorem 4.23 (von Neumann).
Let $\Phi^t : \Omega \to \Omega$ be a measure-preserving flow on a completely metrizable probability space (Ω, Σ, μ) with pure point spectrum. Then, Φ^t is metrically isomorphic to a translation on a compact abelian group $\mathcal{G}$. Explicitly, $\mathcal{G}$ can be chosen as the character group of the point spectrum $\sigma_p(V)$.

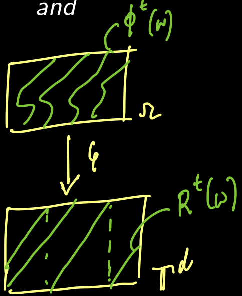
Metric isomorphisms

Corollary 4.24.
If $\sigma_p(V)$ is finitely generated, then Φ^t is metrically isomorphis~~m~~c to an ergodic rotation on the d-torus, where d is the number of generating frequencies of $\sigma_p(V)$. Explicitly, supposing that $\{i\alpha_1, \ldots, i\alpha_d\}$ is a minimal generating set of $\sigma_p(V)$ with corresponding unit-norm eigenfunctions $z_1, \ldots, z_d$ we have

$$R^t \circ \varphi = \varphi \circ \Phi^t,$$

where $R^t : \mathbb{T}^d \to \mathbb{T}^d$ is the torus rotation with frequencies $\alpha_1, \ldots, \alpha_d$, and

$$\varphi(\omega) = (z_1(\omega), \ldots, z_d(\omega)), \quad \mu\text{-a.e.}$$



Numerical challenge: $\sigma_p(V)$ is usually dense in $i\mathbb{R}$ (i.e., as long as $d \geq 2$)

Spectral isomorphisms

Definition 4.25.
With the notation of Definition 4.22, let $U_1 : L^2(\mu_1) \to L^2(\mu_1)$ and $U_2 : L^2(\mu_2) \to L^2(\mu_2)$ be the Koopman operators associated with T_1 and T_2, respectively. We say that T_1 and T_2 are spectrally isomorphic if there exists a unitary map $\mathcal{U} : L^2(\mu_1) \to L^2(\mu_2)$ such that

$$U_2 \circ \mathcal{U} = \mathcal{U} \circ U_1.$$

Every metric isomorphism induces a spectral isomorphism, but the converse is not true (if the system is mixing or is of mixed-spectrum type)

Theorem 4.26 (von Neumann).
Two measure-preserving flows with pure point spectra are metrically isomorphic iff they are spectrally isomorphic.

Dynamics-invariant kernels

$$k : \overset{\Omega}{\cancel{M}} \times \overset{\Omega}{\cancel{M}} \to \mathbb{R}, \quad G : L^2(\mu) \to L^2(\mu), \quad Gf = \int_{\cancel{M}\,\Omega} k(\cdot, \omega) f(\omega)\, d\mu(\omega)$$

- k: Bounded, symmetric kernel.
- G is self-adjoint, compact.

$\phi^t \otimes \phi^t : \Omega \times \Omega \to \Omega \times \Omega$

$\phi^t \otimes \phi^t(\omega, \omega') = [\phi^t(\omega), \phi^t(\omega')]$

Proposition 4.27.
If k is invariant under the product flow,

$$k(\Phi^t(\omega), \Phi^t(\omega')) = k(\omega, \omega'), \qquad (*)$$

then G commutes with the Koopman operator,

$$[U^t, G] = U^t G - G U^t = 0.$$

$$GU^t f(\omega) = \int_\Omega k(\omega, \omega') f(\phi^t(\omega'))\, d\mu(\omega') \overset{\text{by } (*)}{=} \int_\Omega k(\phi^t(\omega), \phi^t(\omega')) f(\phi^t(\omega'))\, d\mu(\omega')$$

$$\overset{\text{since } \mu \text{ is } \phi^t\text{-invariant}}{=} \int_\Omega k(\phi^t(\omega), \omega') f(\omega')\, d\mu(\omega') = U^t G f(\omega)$$

Dynamics-invariant kernels

$$k : \overset{\Omega}{\cancel{M}} \times \overset{\Omega}{\cancel{M}} \to \mathbb{R}, \quad G : L^2(\mu) \to L^2(\mu), \quad Gf = \int_{\cancel{M}\,\Omega} k(\cdot, \omega) f(\omega)\, d\mu(\omega)$$

Corollary 4.28.

Every eigenspace W of G with nonzero corresponding eigenvalue is a finite-dimensional, U^t-invariant subspace of H_p, and $V|_W$ is unitarily diagonalizable.

In more detail, suppose that U^t, G commute and the system is ergodic. Let $U^t z = e^{i\omega t} z$ be a Koopman eigenfunction. Then,

$U^t G z = G U^t z = e^{i\omega t} G z \Rightarrow$ Gz is also a Koopman eigenfunction with eigenvalue $e^{i\omega t}$. Since $e^{i\omega t}$ is a simple eigenvalue (by ergodicity), it follows that $Gz = \lambda z$ for some eigenvalue λ of G.

$\Rightarrow$ Eigenspace W of G corresponding to $\lambda \neq 0$ is a union of finitely many eigenspaces of U^t

Kernels from delay-coordinate maps

$$S_Q(\omega, \omega') = \frac{1}{Q} \sum_{q=0}^{Q-1} \left\| X(\Phi^{q\,\Delta t}(\omega)) - X(\Phi^{q\,\Delta t}(\omega')) \right\|^2 .$$

$= \frac{1}{Q} \| X_Q(\omega) - X_Q(\omega') \|^2$

assume $\mathcal{X} = \mathbb{R}^d$

This is an ergodic average of the function $S : \Omega \times \Omega \to \mathbb{R}$ where $S(\omega, \omega') = \| X(\omega) - X(\omega') \|^2$ under the product system on $\Omega \times \Omega$: $S_Q(\omega,\omega') = \frac{1}{Q} \sum_{q=0}^{Q-1} S(\Phi^{q\Delta t}(\omega), \Phi^{q\Delta t}(\omega'))$

By the mean ergodic theorem,

$$S_Q \xrightarrow[Q \to \infty]{} \bar{S},$$

in $L^2(\mu \times \mu)$, where $\bar{S}$ is a $U^t \otimes U^t$ invariant function.

Proposition 4.29.

Fix a continuous kernel shape function $h : \mathbb{R}_+ \to \mathbb{R}_+$. Then:

e.g. $h(u) = \exp(-u/\varepsilon^2)$ for RBF kernel

1. *$\bar{k}(\omega, \omega') := h(\bar{S}(\omega, \omega'))$ satisfies the assumptions of Proposition 4.27.*
2. *$G_Q : L^2(\mu) \to L^2(\mu)$ with*

$$G_Q f = \int_{M\,\Omega} k_Q(\cdot, \omega) f \, d\mu(\omega)$$

integral op. associated with $\bar{k}$

converges to $\bar{G}$ in $L^2(\mu)$ operator norm.

Delay-coordinate maps

$\phi^t : \Omega \to \Omega$

$X : \Omega \to \mathcal{X}$ (covariate/obs. function)

Given $Q \in \mathbb{N}$ define $X_Q : \Omega \to \mathcal{X}^Q$ s.t.

$$X_Q(\omega) = \big(X(\omega),\ X(\phi^{\Delta t}(\omega)),\ \dots,\ X(\phi^{(Q-1)\Delta t}(\omega)) \big)$$

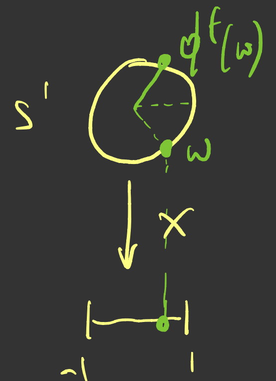
"video"

"snapshots"

Theorem (Takens; Sauer, Yorke, Casdagli; Robinson ...). With "high probability" there is $Q_* \in \mathbb{N}$ s.t. for $Q \geq Q_*$ X_Q is injective

Example: $\phi^t : S^1 \to S^1$ $\phi^t(\omega) = \omega + \alpha t \mod 2\pi$.

$X : S^1 \to \mathbb{R}$ $X(\omega) = \cos \omega$



Suppose that Δt is such that $\phi^{\Delta t}(\omega)$ makes an angle of $\pi/2$ with ω

Then for $Q = 2$,

$$X_2(\omega) = \big(\cos\omega,\ \cos(\phi^{\Delta t}(\omega))\big) = \big(\cos\omega,\ \cos(\omega + \pi/2)\big) = (\cos\omega, \sin\omega)$$

We recover the circle S^1

Finite-difference approximation of the generator

sampling measure on trajectory $\omega_0, \omega_1, \dots, \omega_{N-1}$

Shift operator on $L^2(\mu_N)$

$$V_{\Delta t,N} : L^2(\mu_N) \to L^2(\mu_N), \quad V_{\Delta t,N} = \frac{\tilde V_{\Delta t,N} - \tilde V^*_{\Delta t,N}}{2}, \quad \tilde V_{\Delta t,N} = \frac{\hat U_N - \mathrm{Id}}{\Delta t}$$

antisymmetric operator

Recall $Vf = \lim_{t\to 0} \frac{(U^t - I)f}{t} \approx \frac{1}{\Delta t}(U^{\Delta t} - I)f$

Explicitly, we have

$$\tilde V_{\Delta t,N} f(\omega_n) = \begin{cases} (f(\omega_{n+1}) - f(\omega_n))/\Delta t, & 0 \le n \le N-2, \\ -f(\omega_{N-1})/\Delta t, & n = N-1. \end{cases}$$

Can also define higher-order central, forward, etc., schemes.

Finite-difference approximation of the generator

$$V_{\Delta t,N} : L^2(\mu_N) \to L^2(\mu_N), \; V_{\Delta t,N} = \frac{\tilde{V}_{\Delta t,N} - \tilde{V}^*_{\Delta t,N}}{2}, \; \tilde{V}_{\Delta t,N} = \frac{\hat{U}_N - \mathrm{Id}}{\Delta t}$$

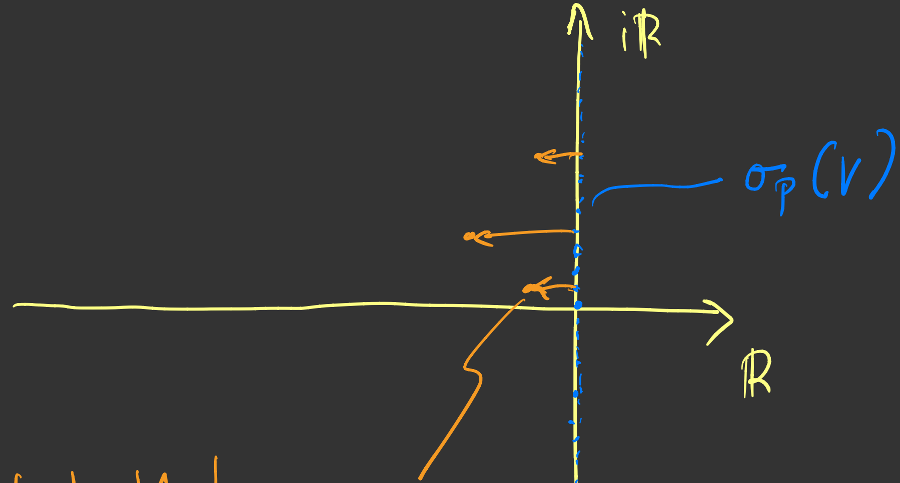
Lemma 4.30.
For $f \in C^1(\Omega)$ and $g \in C(\Omega)$,

$$\lim_{\Delta t \to 0} \lim_{N \to \infty} \langle g, V_{\Delta t,N} f \rangle_{L^2(\mu_N)} = \langle g, Vf \rangle_{L^2(\mu)}.$$

Corollary 4.31.
With the notation of Section 3, if k is C^1, then for every $i, j \in \mathbb{N}$ such that $\lambda_i, \lambda_j \neq 0$,

$$\lim_{\Delta t \to 0} \lim_{N \to \infty} \langle \phi_{i,N} V_{N,\Delta t} \phi_{j,N} \rangle_{L^2(\mu_N)} = \langle \phi_i, V \phi_j \rangle_{L^2(\mu)}.$$

$G_{Q,N} \phi_{i,N} = \lambda_{i,N} \phi_{i,N}$ $\qquad$ $G_Q \phi_i = \lambda_i \phi_i$



Goal:

perturb V by adding a diffusion operator Δ such that the spectrum of $V - \boxed{\varepsilon \Delta}$ becomes discrete

Warning: Singular perturbation

Markov normalization

$$p_\nu(\omega, \omega') = \frac{\tilde{k}(\omega, \omega')}{\rho_\nu(\omega)}, \quad \tilde{k}_\nu(\omega, \omega') = \frac{k(\omega, \omega')}{\sigma_\nu(\omega')},$$

$$\rho_\nu(\omega) = \int_M \tilde{k}_\nu(\omega, \omega')\, d\nu(\omega'), \quad \sigma_\nu(\omega') = \int_M k(\omega', \omega'')\, d\nu(\omega'')$$

- Assume: $k \geq 0$, $k, k^{-1} \in L^\infty(\nu \times \nu)$.
- p is a Markov kernel with respect to ν, i.e.,

$$p \geq 0, \quad \int_{\cancel{M}\,\Omega} p(\omega, \cdot)\, d\nu = 1, \quad \nu\text{-a.e. } \omega \in M.$$

Markov normalization

$$p_\nu(\omega,\omega') = \frac{\tilde{k}(\omega,\omega')}{\rho_\nu(\omega)}, \quad \tilde{k}_\nu(\omega,\omega') = \frac{k(\omega,\omega')}{\sigma_\nu(\omega')},$$
$$\rho_\nu(\omega) = \int_M \tilde{k}_\nu(\omega,\omega')\, d\nu(\omega'), \quad \sigma_\nu(\omega') = \int_M k(\omega',\omega'')\, d\nu(\omega'')$$

Set: $k = k_Q$, $\nu = \mu_N$ or $\nu = \mu$. We get Markov operators $G_{Q,N} : L^2(\mu_N) \to L^2(\mu_N)$, $G_Q : L^2(\mu) \to L^2(\mu)$ with continuous transition kernels:

$$G_{Q,N} f = \int_{\cancel{M}\,\Omega} p_{Q,\mu_N}(\cdot,\omega) f(\omega)\, d\mu_N(\omega), \quad Gf = \int_{\cancel{M}\,\Omega} p_{Q,\mu}(\cdot,\omega) f(\omega)\, d\mu_N(\omega),$$

Large-data limit: As $N \to \infty$, $G_{Q,N}$ converges spectrally to G_Q in the sense of Theorem 3.25.

Markov normalization

$$p_\nu(\omega,\omega') = \frac{\tilde{k}(\omega,\omega')}{\rho_\nu(\omega)}, \quad \tilde{k}_\nu(\omega,\omega') = \frac{k(\omega,\omega')}{\sigma_\nu(\omega')},$$

$$\rho_\nu(\omega) = \int_M \tilde{k}_\nu(\omega,\omega')\, d\nu(\omega'), \quad \sigma_\nu(\omega') = \int_M k(\omega',\omega'')\, d\nu(\omega'')$$

Set: $k = \bar{k}$, $\nu = \mu$. We get a self-adjoint Markov operator $G : L^2(\mu) \to L^2(\mu)$ that commutes with the Koopman operator:

$$\bar{G}f = \int_M \bar{p}_\mu(\cdot,\omega) f(\omega)\, d\mu(\omega).$$

Infinite-delay limit: As $Q \to \infty$ G_Q converges in operator norm, and thus spectrally, to $\bar{G}$.

Remark.
By Corollary 4.28, every eigenfunction ϕ_j of G corresponding to nonzero eigenvalue lies in the domain of the generator V.

Diffusion regularization

$$\Delta : D(\Delta) \to \tilde{H}_p, \quad \Delta = (I - G)^{-1}$$

$$\Delta\phi_j = \eta_j\phi_j, \quad \eta_j = 1 - \frac{1}{\lambda_j}$$

think of G as a heat operator

$G \approx e^{-\tau\Delta}$

Taylor expand

$\frac{1}{I-G} \approx \frac{1}{I-e^{-\tau\Delta}} \approx \tau\Delta$

- $\tilde{H}_p = \overline{\operatorname{ran} G} \subseteq H_p$.
- $D(\Delta) \equiv \tilde{H}^2_p = \{f \in \tilde{H}_p : \sum_j \eta_j |\langle \phi_j, f\rangle_{L^2(\mu)}|^2 < \infty\}$.

Proposition 4.32.

1. *For every* $\epsilon > 0$,
$$\mathcal{L}_\epsilon = V - \epsilon\Delta,$$
is a well-defined dissipative operator on $\tilde{H}^2_p$, *i.e.,* $\operatorname{Re}\langle f, \mathcal{L}_\epsilon f\rangle \leq 0$.
2. *Let* z *be an eigenfunction of* V *lying in* H^2_p *with corresponding eigenvalue* $i\omega$. *Then, we have*

$$\Delta z = \eta z, \quad \mathcal{L}_\epsilon z = \gamma z, \quad \gamma = -\epsilon\eta + i\omega.$$

↳ Eigenvalues of $\mathcal{L}_\varepsilon$ are equal to eigenfrequencies $i\omega$ shifted by $-\varepsilon\eta$

Petrov-Galerkin method

Infinite-dimensional variational problem

Find $z_j \in \tilde{H}_p^2$ and $\gamma_j \in \mathbb{C}$, such that for all $f \in \tilde{H}_p$,

$$\langle f, V z_j \rangle_{L^2(\mu)} - \epsilon \langle f, \Delta z \rangle_{L^2(\mu)} = \gamma_j \langle f, z \rangle_{L^2(\mu)}.$$

- The above is a well-defined variational eigenvalue problem, i.e., it satisfies the appropriate boundedness and coercivity conditions.
- We order the solutions z_j in order of increasing Dirichlet energy,

$$E_j = \langle z_j, \Delta z_j \rangle_{L^2(\mu)} = \operatorname{Re} \gamma_j / \epsilon.$$

Petrov-Galerkin method

Data-driven approximation

Find $z_j \in \tilde{H}^2_{p,L,Q,N}$ *and* $\gamma_j \in \mathbb{C}$*, such that for all* $f \in \tilde{H}_{p,L,Q,N}$*,*

$$\langle f, Vz_j \rangle_{L^2(\mu_N)} - \epsilon \langle f, \Delta z_j \rangle_{L^2(\mu_N)} = \gamma_j \langle f, z_j \rangle_{L^2(\mu_N)}.$$

matrix generalized eigenvalue problem

- $\tilde{H}_{p,L,Q,N} = \mathrm{span}\{\phi_{0,Q,N}, \dots, \phi_{L-1,Q,N}\} \subseteq L^2(\mu_N)$, where $\phi_{j,Q,N}$ are eigenfunctions of $G_{Q,N}$.
- $H^2_{p,L,Q,N}$ defined analogously to $\tilde{H}^2_p$.
- The data-driven scheme converges in the iterated limit

$$\lim_{L\to\infty} \lim_{Q\to\infty} \lim_{\Delta t\to 0} \lim_{N\to\infty}.$$

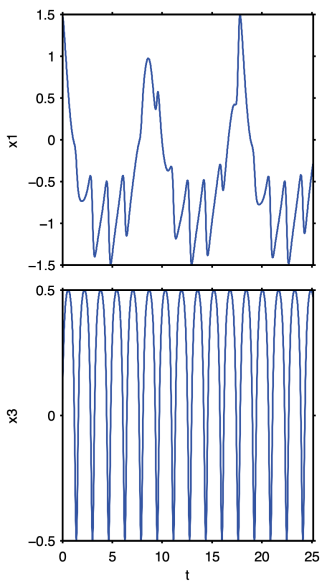
$z_j = \sum_{i=1}^{L} c_i \phi_i$

$f = \sum_{i=1}^{L} d_i \phi_i$

Get matrix eigenvalue problem

$A\vec{c} = \gamma B \vec{c}$

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

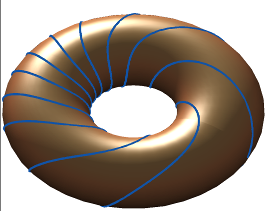


$$\dot{\omega}(t) = \vec{V}(\omega(t))$$

$$\vec{V}(\omega) = (V_1, V_2), \quad \omega = (\theta_1, \theta_2)$$

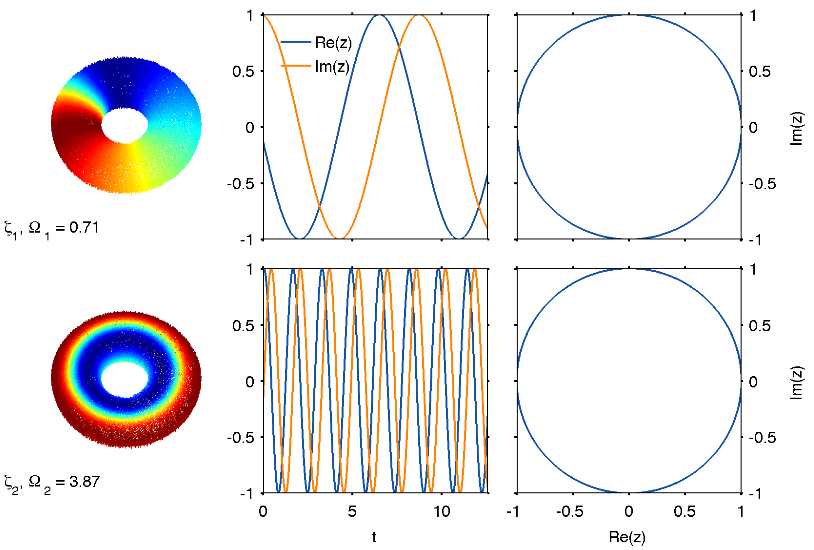
$$V_1 = 1 + \beta \cos \theta_1$$

$$V_2 = \alpha(1 - \beta \sin \theta_2)$$

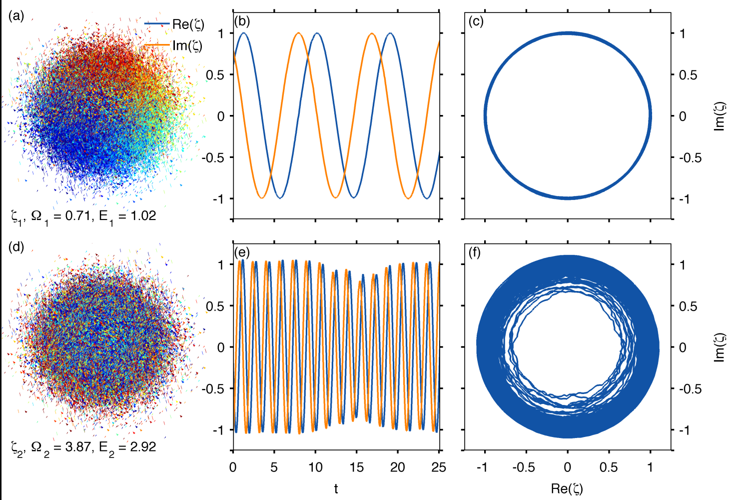


$\alpha = \sqrt{30}$, $\beta = \sqrt{1/2}$

Koopman eigenfunctions



Koopman eigenfunctions from noisy data



Koopman eigenfunctions for the variable-speed flow on $\mathbb{T}^2$ recovered from data from data corrupted with i.i.d. Gaussian noise in $\mathbb{R}^3$ with SNR $\simeq 1$.

Approximate Koopman eigenfunctions

Definition 4.33.
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

$$\|U^t z - \nu_t z\|_{L^2(\mu)} < \epsilon \|z\|_{L^2(\mu)}. \qquad (*)$$

- A Koopman eigenfunction is an ϵ-approximate eigenfunction for every $\epsilon > 0$.
- We seek $z \in L^2(\mu)$ which is an ϵ-approximate eigenfunction for "small" ϵ, and t lying in a "large" time interval.

It can be shown that $\| [U^t, G_Q] \| \leq \frac{C}{Q}$

$\Rightarrow$ G_Q has approximately Koopman-invariant eigenspaces.
Look for elements of these eigenspaces as candidates of observables z satisfying $(*)$

Approximate eigenfunctions from delay-coordinate maps

Theorem 4.34.
Let ϕ and ψ be mutually-orthogonal, unit-norm, real eigenfunctions of G_Q corresponding to nonzero eigenvalues κ and λ, respectively, with $\kappa \geq \lambda$. Assume that κ, λ are simple if distinct and twofold-degenerate if equal. Define

$$z = \frac{1}{\sqrt{2}}(\phi + i\psi), \quad \alpha_t = \langle z, U^t z \rangle, \quad \nu = \langle \psi, V\phi \rangle,$$

where ω is real, and set $T = (Q-1)\,\Delta t$, $\delta_T = (\kappa - \lambda)/\sqrt{2}$, $\tilde{\delta}_T = \delta_T/\kappa$,

$$\gamma_T = \min_{u \in \sigma(G_Q) \setminus \{\kappa, \lambda\}} \{\min\{|\kappa - u|, |\lambda - u|\}\}.$$

Then, the following hold for every $t \geq 0$:

Approximate eigenfunctions from delay-coordinate maps

Theorem 4.34.

1. *α_t lies in the $\tilde{\epsilon}_t$-approximate point spectrum of U^t, and z is a corresponding $\tilde{\epsilon}_t$-approximate eigenfunction for the bound*

$$\tilde{\epsilon}_t = s_t + \sqrt{S_t},$$

where

$$s_t = \frac{1}{\gamma_T}\left(\frac{C_1 t}{T} + 3\delta_T\right), \quad S_t = \frac{C_2(1+\tilde{\delta}_T)}{\lambda}\int_0^t s_u \, du.$$

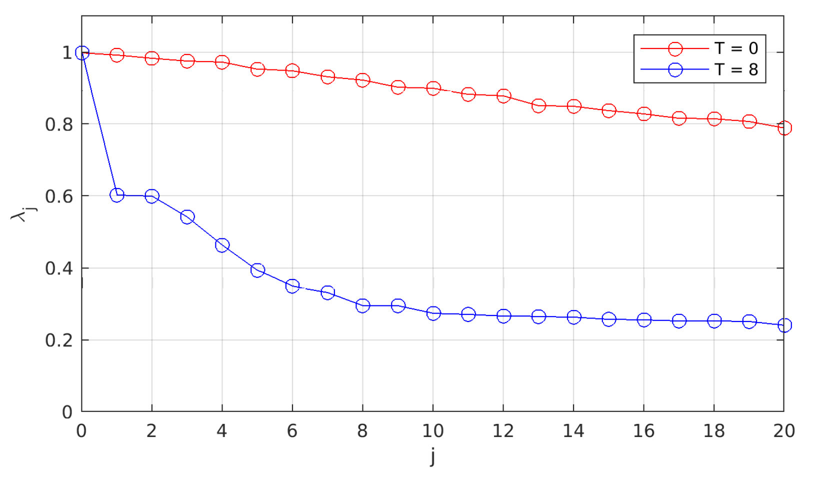
↳ length of delay embedding window $= Q\Delta t$

Here, C_1 and C_2 are constants that depend only on the observation map F and generator V.

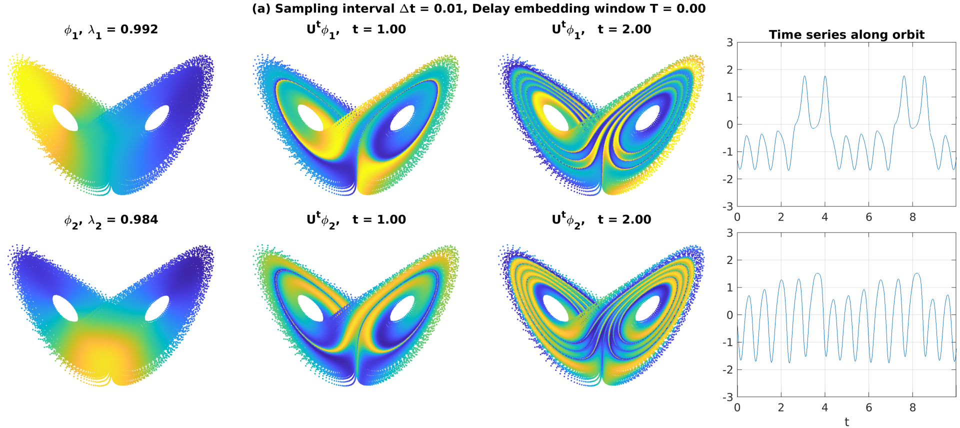
2. *The modulus $|\nu|$ is independent of the choice of the real orthonormal basis $\{\phi, \psi\}$ for the eigenspace(s) corresponding to κ and λ. Moreover, the phase factor $e^{i\nu t}$ is related to the autocorrelation function α_t according to the bound*

$$|\alpha_t - e^{i\nu t}| \leq 2\sqrt{S_t}.$$

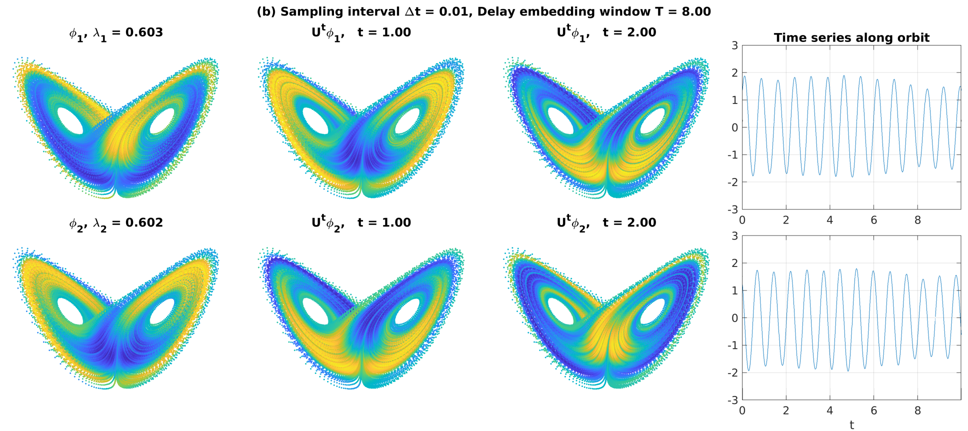
Application to L63 system



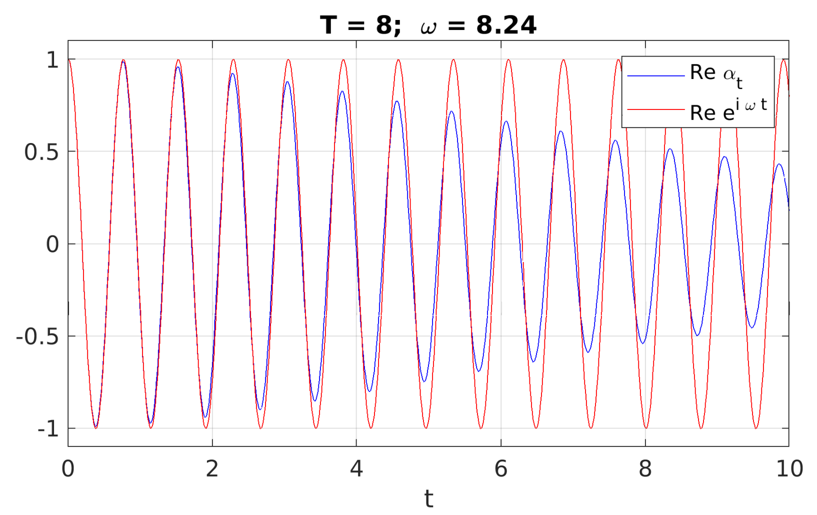
Application to L63 system



Application to L63 system



Application to L63 system

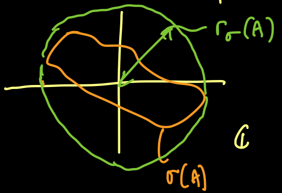


Spectrum

Definition 4.35.
Let $A : D(A) \to F$ be a densely-defined operator on a Banach space F over $\mathbb{C}$ with domain $D(A) \subseteq F$.

1. The spectrum of A, denoted as $\sigma(A)$ is the set of complex numbers λ such that $A - \lambda I$ has no bounded inverse.
2. The resolvent set of A, denoted as $\rho(A)$, is the complement of $\sigma(A)$ in $\mathbb{C}$.
3. For every $\lambda \in \rho(A)$ the resolvent $R_A(\lambda)$ is the bounded operator given by $\cancel{\rho(A)}\, R_A(\lambda) = (A - \lambda I)^{-1}$.
4. The spectral radius of A is defined as $r_\sigma(A) = \sup_{\lambda\in\sigma(A)} \cancel{|\lambda|}\, |\lambda|$.

There is no bounded operator $B : F \to F$ s.t. $BA = I$ on $D(A)$
$ABf = f$ for $f \in F$ s.t. $Bf \in D(A)$



Spectrum

Theorem 4.36.
With the notation of Definition 4.35, the following hold.

1. *$\sigma(A)$ is a closed subset of $\mathbb{C}$.*
2. *If A is not closed, then $\sigma(A) = \mathbb{C}$.*
3. *$\underbrace{\text{If } D(A) = F \text{ and } A \text{ is bounded,}}_{\text{and thus } A \text{ is closed}}$ then $r_\sigma(A) \le \|A\|$.*

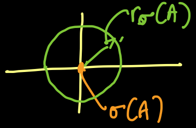
The spectrum is "interesting" only for closed operators

Example: $F = \mathbb{C}^2$

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\|A\| = 1$$

$$\sigma(A) = \sigma_p(A) = \{0\}$$



DECOMPOSITION OF THE SPECTRUM

Assume A is closed

$\lambda \in \sigma(A) \Leftrightarrow \{A - \lambda I \text{ has no bd. inverse}\} \Leftrightarrow A$ is not bijective

$A - \lambda I$ is not injective $\Leftrightarrow \ker A - \lambda I \neq \{0\}$

$\Leftrightarrow \lambda \in \sigma_p(A)$ (λ is an eigenvalue)

$A - \lambda I$ is injective but not surjective

ran $A - \lambda I$ is a dense subspace of F

$\lambda \in \sigma_{pc}(A)$ (purely continuous)

$\Downarrow$

$A - \lambda I$ is not bounded below

$\exists$ a sequence $f_1, f_2, \ldots$ with $\|f_n\|_F = 1$

s.t. $\|(A - \lambda I) f_n\| \to 0$

ran$(A - \lambda I)$ is not dense

$\lambda \in \sigma_r(A)$ (residual)

For self-adjoint and skew-adjoint ops. $\sigma_r(A) = \emptyset$.

Projection-valued measures (spectral measures)

Definition 4.37.
Let $(H, \langle \cdot, \cdot \rangle_H)$ be a Hilbert space over $\mathbb{C}$. A map $E : \mathfrak{B}(\mathbb{C}) \to B(H)$ is called a projection-valued measure (PVM) if:

1. For every $S \in \mathfrak{B}(\mathbb{C})$, $E(S)$ is an orthogonal projection. $E(S)^2 = E(S)$, $E(S)^* = E(S)$
2. $E(\mathbb{C}) = I$.
3. For every $f, g \in H$, the map $\varepsilon_{fg} : \mathfrak{B}(\mathbb{C}) \to \mathbb{C}$ with

$$\varepsilon_{fg}(S) = \langle f, E(S)g \rangle_H$$

is a complex measure.

Example $H = \mathbb{C}^n$, A : self-adjoint $n \times n$ matrix.
We know that $\sigma(A) = \{\lambda_1, \dots, \lambda_n : \lambda_j \in \mathbb{R}$ is an e-value of $A\}$ with multiplicities and there exists an orthonormal basis $\{u_1, \dots, u_n\}$ of $\mathbb{C}^n$ s.t. $Au_j = \lambda_j u_j$. Then,
Define $\Pi_j \in B(H)$ s.t. $\Pi_j v = \langle u_j, v \rangle_{\mathbb{C}^n} u_j$ (orthogonal projection).
$E : \mathcal{B}(\mathbb{C}) \to B(H)$ s.t. $E(S) = \sum_{j : \lambda_j \in S} \Pi_j$ is a PVM.

Projection-valued measures

Functional calculus

Theorem 4.38.
With the notation of Definition 4.37, let $f : \mathbb{C} \to \mathbb{C}$ be a Borel-measurable function. Then, there exists a unique operator $E_f : D(E_f) \to H$ with domain

$$D(E_f) = \left\{ h \in H : \int_{\mathbb{C}} |f|^2 \, d\varepsilon_{hh} < \infty \right\},$$

such that

$$\langle g, E_f h \rangle_H = \int_{\mathbb{C}} f \, d\varepsilon_{gh}, \quad \forall g \in H, \quad \forall h \in D(E_f).$$

For the self-adjoint matrix in the previous example, given a function $f : \mathbb{C} \to \mathbb{C}$ we can define $f(A)$ as

$$f(A) = \sum_j f(\lambda_j) \Pi_j$$

Notation.

- $\int_{\mathbb{C}} f \, dE \equiv \cancel{E_f}\, f_E$.
- If $A = \int_{\mathbb{C}} \mathrm{Id} \, dE$, then $f(A) \equiv \cancel{E_f}\, f_E$.

Matrix example $A = \sum_j \lambda_j \Pi_j = \int_{\mathbb{C}} \lambda \, dE(\lambda)$

Spectral theorem for skew-adjoint operators

Theorem 4.39.
Let $A : D(A) \to H$ be skew-adjoint.

1. *$\sigma(A)$ is a subset of the imaginary line.*
2. *There exists a unique PVM $E_A : \mathfrak{B}(\mathbb{C}) \to \mathbb{C}$ such that*
$$A = \int_{\mathbb{R}} i\alpha \, dE_A(\alpha).$$
3. *$i \operatorname{supp} E_A = \sigma(A)$.*
4. *If $\{U^t : H \to H\}_{t\in\mathbb{R}}$ is the C_0 unitary group generated by A, then*
$$U^t = e^{tA} \equiv \int_{\mathbb{R}} e^{i\alpha t} \, dE_A(\alpha).$$

Unitary Koopman evolution group

$$U^t : L^2(\mu) \to L^2(\mu), \quad U^t f = f \circ \Phi^t, \quad U^{t*} = U^{-t}$$

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

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

Spectral measure: $E : \mathfrak{B}(\mathbb{R}) \to B(L^2(\mu))$,

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

Unitary Koopman evolution group

$$U^t : L^2(\mu) \to L^2(\mu), \quad U^t f = f \circ \Phi^t, \quad U^{t*} = U^{-t}$$

Theorem 4.40.
There is a U^t-invariant orthogonal splitting $L^2(\mu) = H_p \oplus H_c$ such that:

1. *H_p has an orthonormal basis $\{z_j\}$ consisting of eigenfunctions of the generator,*

$$V z_j = i\alpha_j z_j, \quad \alpha_j \in \mathbb{R}.$$

2. *For every $f \in H_c$ and $g \in L^2(\mu)$,*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |\langle g, U^t f\rangle_{L^2(\mu)}| \, dt = 0.$$

3. *$E = E_p + E_c$, where:*
   - *E_p is a purely atomic measure taking values in $B(H_p)$.*
   - *E_c is a continuous measure taking values in $B(H_c)$.*

→ $E_c(\{\lambda\}) = 0$
For any $f, g \in L^2(\mu)$, the function
$\lambda \mapsto \langle f, E_c((-\infty, \lambda])g\rangle_{L^2(\mu)}$
is continuous

↳ The atoms of E_p, i.e., the Borel sets S s.t. $E_p(S') = 0$ for any $S' \subset S$, are singleton sets consisting of the eigenvalues of V and $E_p(\{i\alpha_j\}) = \Pi_j$ where $\Pi_j f = \langle z_j, f\rangle_{L^2(\mu)} z_j$ is the orthogonal projection onto the corresponding eigenspace.

Compactification schemes for the Koopman generator

Given:

Positive-definite, C^1 kernel $k : \Omega \times \Omega \to \mathbb{R}$.

Integral operators $K : L^2(\mu) \to \mathcal{K}$, $G = K^* K$.

RKHS

Pre-smoothing:

$$A : L^2(\mu) \to L^2(\mu), \quad A = VG.$$

- $\operatorname{ran} G \subseteq \operatorname{ran} K^* \subset D(V)$.
- $A = VG$ is a Hilbert-Schmidt integral operator on $L^2(\mu)$ with kernel $k' \in C(X \times X)$, $k'(\cdot, \omega) = Vk(\cdot, \omega)$, i.e.,

$$Af = \int_\Omega k'(\cdot, \omega) f(\omega)\, d\mu(\omega).$$

Compactification schemes for the Koopman generator

Given:

Positive-definite, C^1 kernel $k : \Omega \times \Omega \to \mathbb{R}$.

Integral operators $K : L^2(\mu) \to \mathcal{K}$, $G = K^* K$.

Post-smoothing:

$$B : L^2(\mu) \to L^2(\mu), \quad B = \overline{GV}.$$

- $GV \subset (GV)^{**} = B = -A^*$.
- B is a Hilbert-Schmidt integral operator with

$$Bf = -\int_\Omega k'(\cdot, \omega) f(\omega) \, d\mu(\omega).$$

Compactification schemes for the Koopman generator

Given:

Positive-definite, C^1 kernel $k : \Omega \times \Omega \to \mathbb{R}$.

Integral operators $K : L^2(\mu) \to \mathcal{K}$, $G = K^* K$.

Skew-adjoint compactification on the RKHS:

$$W : \mathcal{K} \to \mathcal{K}, \quad W = KVK^*.$$

$W^* = -W$

- W is a skew-adjoint, Hilbert-Schmidt operator on $\mathcal{K}$ satisfying

$$Wf = -\int_\Omega k'(\omega, \cdot) f(\omega)\, d\mu(\omega).$$

Compactification schemes for the Koopman generator

Given:

Positive-definite, C^1 kernel $k : \Omega \times \Omega \to \mathbb{R}$.

Integral operators $K : L^2(\mu) \to \mathcal{K}$, $G = K^* K$.

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

$$\tilde{V} : L^2(\mu) \to L^2(\mu), \quad \tilde{V} = G^{1/2} V G^{1/2}.$$

- $K = \mathcal{U} G^{1/2}$ (polar decomposition).
- $\tilde{V}$ is a skew-adjoint, Hilbert-Schmidt operator on $L^2(\mu)$ related to W by
$$\tilde{V} = \mathcal{U}^* W \mathcal{U}.$$

Eigenvalues and eigenfunctions

Proposition 4.41.

Let $k : \Omega \times \Omega \to \mathbb{R}$ be a C^1, L^2-universal, μ-Markov ergodic kernel.

1. *There exists an orthonormal basis $\tilde{z}_0, \tilde{z}_1, \dots,$ of $L^2(\mu)$ consisting of eigenfunctions of $\tilde{V}$,*

$$\tilde{V}\tilde{z}_j = i\alpha_j \tilde{z}_j, \quad \alpha_j \in \mathbb{R}.$$

2. *In the above, $i\alpha_0 = 0$ is a simple eigenvalue corresponding to the constant eigenfunction $\tilde{z}_0 = 1$.*
3. *$\tilde{V}$ has an associated purely atomic PVM $\tilde{E} : \mathfrak{B}(\mathbb{R}) \to B(L^2(\mu))$ such that*

$$\tilde{E}(S) = \sum_{j:\alpha_j \in S} \underbrace{\langle \tilde{z}_j, \cdot \rangle_{L^2(\mu)} \tilde{z}_j}_{\Pi_j}, \quad \tilde{V} = \int_{\mathbb{R}} i\alpha \, d\tilde{E}(\alpha).$$

$$= \sum_j i\alpha_j \Pi_j$$

Strong resolvent convergence

Definition 4.42.

1. A one-parameter family of operators $A_\tau : D(A_\tau) \to H$, $\tau > 0$, on a Hilbert space H is said to converge to a skew-adjoint operator $A : D(A) \to H$ in strong resolvent sense if for every $\rho \in \mathbb{C} \setminus \{i\mathbb{R}\}$ in the resolvent set of A the resolvents $(A_\tau - \rho)^{-1}$ converge to $(A - \rho)^{-1}$ strongly.
2. The family A_τ is said to be *p*2-continuous if it is uniformly bounded and $\tau \mapsto \|p(A_\tau)\|$ is continuous for every degree-2 polynomial p.
3. If A_τ is skew-adjoint, A_τ is said to converge to A in strong dynamical sense if for every $t \in \mathbb{R}$, e^{tA_τ} converges to e^{tA} strongly.

Strong resolvent convergence

Theorem 4.43.
With the notation of Definition 4.42, suppose that A_τ is skew-adjoint. Then:

1. *Strong resolvent convergence is equivalent to strong dynamical convergence.*
2. *A sufficient condition for strong resolvent convergence $A_\tau \to A$ is that A_τ converges to A strongly in a core, i.e., a subspace $C \subseteq D(A)$ such that $\overline{A|_C} = A$.*
3. *The domain $D(A^2)$ is a core for A.*

Strong resolvent convergence

Theorem 4.44.
Let $A_\tau : D(A_\tau) \to H$ be a one-parameter family of skew-adjoint operators that converges to a skew-adjoint operator $A : D(A) \to H$ in strong resolvent sense. Let $E_\tau : \mathfrak{B}(R) \to B(H)$ and $E : \mathfrak{B}(R) \to B(H)$ be the PVMs associated with A_τ and A, respectively.

1. *For every bounded, Borel-measurable set $\Omega \subset R$ such that $E(\partial\Omega) = 0$, $E_\tau(\Omega)$ converges strongly to $E(\Omega)$.*
2. *For every bounded, continuous function $Z : i\mathbb{R} \to \mathbb{C}$, $Z(A_\tau)$ converges strongly to $Z(A)$.*
3. *If the operators A_τ are compact, then for every element $i\alpha \in i\mathbb{R}$ of the spectrum of A there exists a one-parameter family $i\alpha_\tau$ of eigenvalues of A_τ such that $\lim_{\tau\to 0} \alpha_\tau = \alpha$. Moreover, if A_τ is p2-continuous, the curve $\tau \mapsto \alpha_\tau$ is continuous.*

Spectral convergence of the compactified generators

Theorem 4.45.
Let $\{G_\tau\}_{\tau \geq 0}$ be a strongly continuous, ergodic semigroup of Markov operators on $L^2(\mu)$ such that for every $\tau > 0$,

$$G_\tau f = \int_\Omega k_\tau(\cdot, \omega) f(\omega) \, d\mu(\omega),$$

where $k_\tau : \Omega \times \Omega \to \mathbb{R}$ is a C^1, L^2-universal, positive-definite kernel. Then, Theorem 4.44 holds for the compactified generators

$$\tilde{V}_\tau = G_\tau^{1/2} V G_\tau^{1/2}.$$

Construction of the semigroup G_τ

1. Start from an L^2-universal, C^1 kernel $\kappa : \Omega \times \Omega \to \mathbb{R}$.
2. Normalize κ to an L^2-universal, C^1, bistochastic Markov kernel $p : \Omega \times \Omega \to \mathbb{R}$ (Coifman & Hirn '13). Let $P : L^2(\mu) \to L^2(\mu)$ be the associated integral operator.
3. Define the Laplace-like operator $\Delta = (I - P)^{-1}$.
4. Define $G_\tau = e^{-\tau\Delta}$.

Dirichlet energy

$$P\phi_j = \lambda_j \phi_j, \quad \lambda_j > 0, \quad \langle \phi_i, \phi_j \rangle_{L^2(\mu)} = \delta_{ij}$$
$$G_\tau \phi_j = \lambda_{j,\tau} \phi_j, \quad \lambda_{j,\tau} = e^{-\tau \eta_j}, \quad \eta_j = 1 - \frac{1}{\lambda_j}.$$

- $\mathcal{H}$: RKHS associated with p.
- $f \in L^2(\mu)$ has a representative in $\mathcal{H}$ iff

$$\tilde{\mathcal{D}}(f) := \sum_{j=0}^{\infty} \frac{|\langle \phi_j, f \rangle_{L^2(\mu)}|^2}{\lambda_j} < \infty.$$

- For every such (nonzero) f, we define the Dirichlet energy

$$\mathcal{D}(f) = \frac{\tilde{\mathcal{D}}(f)}{\|f\|^2_{L^2(\mu)}} - 1.$$

Coherent observables

$$W_\tau = K_\tau V K_\tau^*$$

$$W_\tau \zeta_{j,\tau} = i\omega_{j,\tau}\zeta_{j,\tau}, \quad z_{j,\tau} = \frac{K_\tau^* \zeta_{j,\tau}}{\|K_\tau^* \zeta_{j,\tau}\|_{L^2(\mu)}}.$$

Proposition 4.46.

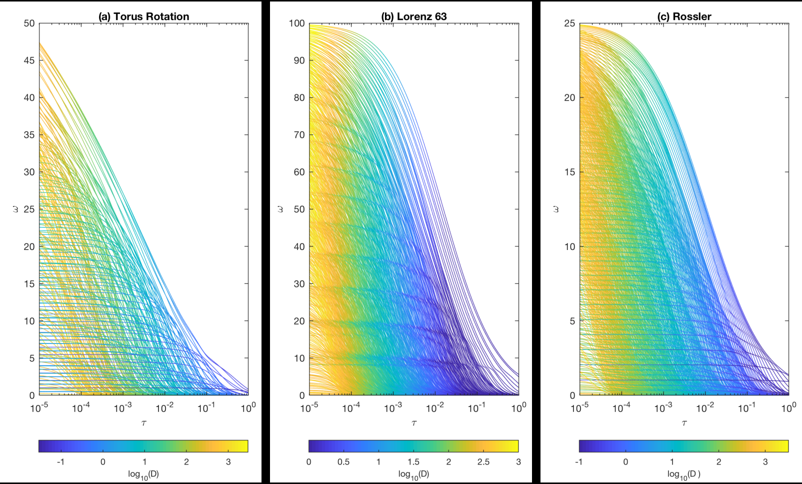
There exists a continuous function $R(\epsilon, \tau)$ that diverges as $\tau \to 0$ for every $\epsilon > 0$ such that

$$\|U^t z_{j,\tau} - e^{i\omega_{j,\tau}} z_{j,\tau}\|_{L^2(\mu)} < \epsilon, \quad |t| \leq T(\epsilon, \tau) := \frac{R(\epsilon, \tau)}{\sqrt{\mathcal{D}(z_{j,\tau}) + 1}}.$$

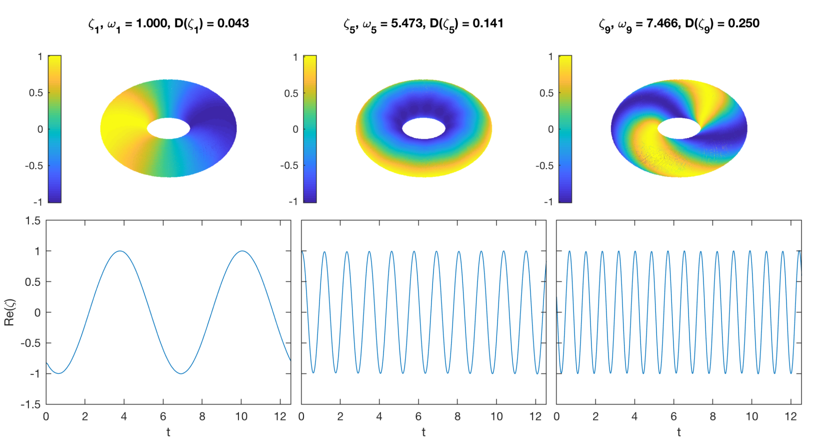
Moreover:

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

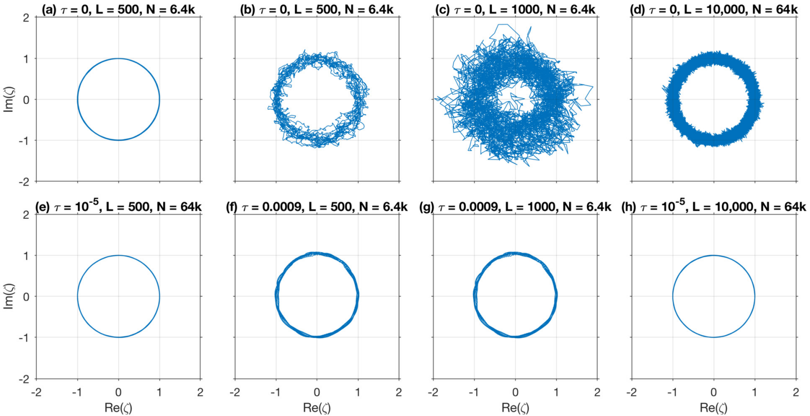
Numerical examples



Torus rotation—eigenfunctions of W_τ

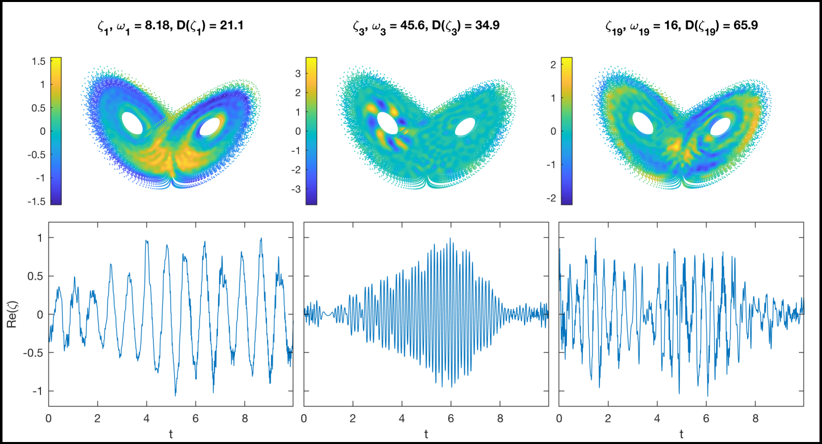


Torus rotation

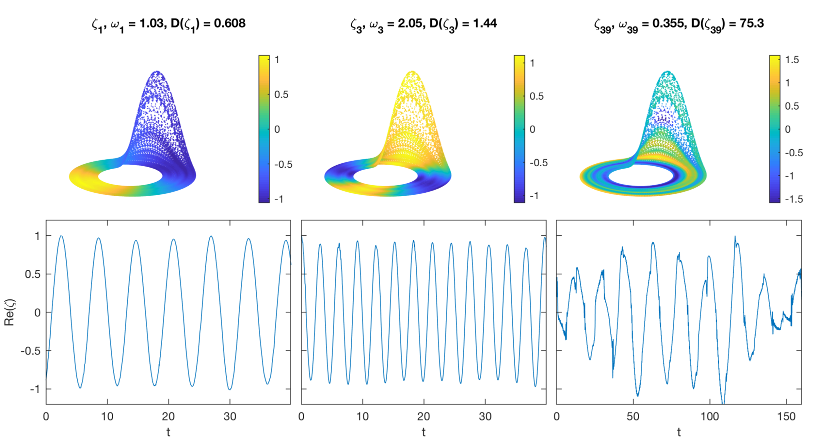


Due to the density of the spectrum in the imaginary line, regularization is important, even for a system with pure point spectrum.

L63 system—eigenfunctions of W_τ



Rössler system—eigenfunctions of W_τ



Further reading

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