Koopman Operators and Dynamic Mode Decomposition

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- The abstract dynamical system is specified by the pair (M, T)

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$$\mu(S) = \mu(T^{-1}S)$$

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- Track: $f(p) \to f(T(p)) \to f(T^2(p)) \to f(T(p^3)) \dots$
- Can describe the dynamics as:

$$p_{n+1} = T(p_n) \text{ and } v_n = f(p_n)$$

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- Generally U is infinite-dimensional

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- $f_1, \ldots, f_K$ could be physically relevant observables or part of the function basis for $\mathcal{F}$

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- More generally: $F : M \to V$ where V is a vector space

Koopman Operators in Continuous Time D.S.

- Consider the continuous time dynamical system

$$\dot{p} = T(p)$$

Example: Cyclic Group

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- Let $\mathcal{F}$ be $\mathbb{C}$-valued functions on M
- Space of observables is $\mathbb{C}^3$

Setup

- Let f_1, f_2, f_3 be indicator functions on e, a, a^2:

$$f_1(p) = \begin{cases} 1 & \text{if } p = e \\ 0 & \text{if } p \neq e \end{cases}$$

$$f_2(p) = \begin{cases} 1 & \text{if } p = a \\ 0 & \text{if } p \neq a \end{cases}$$

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- Form a basis for $\mathcal{F}$

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- Action of the Koopman operator on this basis:

$$[Uf_1](p) = f_1(a \cdot p) = f_3(p)$$
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- Consider arbitrary observable $f \in \mathcal{F}$ i.e. $f = c_1 f_1 + c_2 f_2 + c_3 f_3$
- Consider the action of the Koopman operator on f:

$$Uf = U(c_1 f_1 + c_2 f_2 + c_3 f_3) = c_1 f_3 + c_2 f_1 + c_3 f_2$$

Example: Cyclic Group

- Matrix representation of the Koopman operator U in the $\{f_1, f_2, f_3\}$ basis:

$$U \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

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- Let $\mathcal{F}$ denote space of functions $\mathbb{R}^d \to \mathbb{C}$
- Let $\{\mathbf{b}_1 \ldots, \mathbf{b}_d\} \subset M$ be a basis for M; define $f_i(x) = \langle \mathbf{b}_i, x \rangle$

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- The action of the Koopman operator $U : \mathcal{F} \to \mathcal{F}$ on f_i is

$$[Uf_i](x) = \langle b_i, T(x) \rangle = \begin{bmatrix} b_{i,1} & \dots & b_{i,d} \end{bmatrix} \begin{bmatrix} \mu_1 x_1 \\ \vdots \\ \mu_d x_d \end{bmatrix}$$

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- This is the action of the Koopman operator on the particular observable F, not the entire observable space $\mathcal{F}$

Example: Heat equation with periodic boundary conditions

Mode Analysis

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- Assume: U is a bounded, continuous operator on $\mathcal{F}$

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- λ's are the eigenvalues of the generator U, and $\{e^{\lambda_i}\}$ of the Koopman semi-group

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- $\implies$ set of eigenfunctions forms an abelian semigroup under pointwise products of functions
- Concretely: If $\phi_1, \phi_2 \in \mathcal{F}$ are eigenfunctions of U with eigenvalues λ_1 and λ_2, then $\phi_1\phi_2$ is an eigenfunction of U with eignevalue $\lambda_1\lambda_2$

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- If ϕ is an eigenfunction that vanishes nowhere and $r \in \mathbb{R}$, then ϕ^r is an eigenfunction with eigenvalue λ^r
- Eigenfunctions that vanish nowhere form an Abelian group

Spectral Equivalence of Topologically Conjugate Systems

Proposition

Let $S : M \to M$ and $T : N \to N$ be topologically conjugate; i.e. $\exists$ a homomorphism $h : N \to M$ such that $S \circ h = h \circ T$. If ϕ is an eigenfunction of U_S with eigenvalue λ, then $\phi \circ h$ is an eigenfunction of U_T at eigenvalue λ

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- Maps Λ and T are topologically conjugate by $\Lambda V^{-1} = V^{-1}T$

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- T is a matrix with eigenvectors v_1, v_2 at eigenvalues λ_1, λ_2 with $v_i \neq e_j$
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$$\begin{bmatrix} x_1^{(k+1)} \\ x_2^{(k+1)} \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \begin{bmatrix} x_1^{(k)} \\ x_2^{(k)} \end{bmatrix} := \Lambda \begin{bmatrix} x_1^{(k)} \\ x_2^{(k)} \end{bmatrix}$$

- Maps Λ and T are topologically conjugate by $\Lambda V^{-1} = V^{-1}T$
- V^{-1} is now the h from the proposition

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- Likewise

$$[U^m f](p) = \sum_{i=1}^{n} \lambda_i^m c_i(f)\phi_i(p)$$

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Koopman Mode

Definition

Let ϕ_i be an eigenfunction for the Koopman operator corresponding to eigenvalue λ_i. For a vector valued observable $F : M \to V$, the Koopman mode $C_i(F)$, corresponding to ϕ_i is the vector of coefficients of the projection of F onto $span\{\phi_i\}$

Computation of Koopman Modes: Theory

Theorem (Yosida)

Let $\mathcal{F}$ be a Banach space and $U : \mathcal{F} \to \mathcal{F}$. Assume $\|U\| \leq 1$. Let λ be an eigenvalue of U such that $|\lambda| = 1$. Let $\tilde{U} = \lambda^{-1}U$, and define:

$$A_K(\tilde{U}) = \frac{1}{K}\sum_{k=0}^{K-1} \tilde{U}^k$$

Then A_K converges in the strong operator topology to the projection operator on the subspace of U-invariant function; i.e. onto the eigenspace E_λ corresponding to λ. That is, for all $f \in \mathcal{F}$,

$$\lim_{K\to\infty} A_K f = \lim_{K\to\infty} \frac{1}{K}\sum_{k=0}^{K-1} \tilde{U}^k f = P_\lambda f$$

where $P_\lambda : \mathcal{F} \to E_\lambda$ is a projection operator.

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- Consider the case when the eigenvalues are simple and $|\lambda_1| = \cdots = |\lambda_\ell| = 1$ and $|\lambda_n| < 1$ for $n > \ell$

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- Previous theorem reduces to Fourier analysis for those eigenvalues on the unit circle.
- When an observable is a linear combination of a finite collection of eigenfunctions corresponding to simple eigenvalues, we have an extension of the previous theorem

Theorem (Generalized Laplace Analysis)

Let $\{\lambda_1, \dots, \lambda_m\}$ *be a finite set of simple eigenvalues for* U*, ordered so that* $|\lambda_1| \geq \cdots \geq |\lambda_m|$ *and let* ϕ_i *be an eigenfunction corresponding to* λ_i*. For each* $n \in \{1, \dots, N\}$*, assume* $f_n : M \to \mathbb{C}$ *and* $f_n \in span\{\phi_1, \dots, \phi_m\}$*. Define the vector-valued observable* $F = (f_1, \dots, f_N)^T$*. Then the Koopman modes can be computed via:*

$$\phi_j C_j(F) = \lim_{K \to \infty} \frac{1}{K} \sum_{k=0}^{K-1} \lambda_j^{-k} \left[U^k F - \sum_{i=1}^{j-1} \lambda_i^k \phi_i C_i(F) \right]$$

- A simple consequence of the theorem of Yosida

A Numerical Algorithm: Dynamic Mode Decomposition

Introduction

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- Data driven approach: Have a sequence of observations of a vector-valued observable along a trajectory $\{T^k p\}$
- Dynamic mode decomposition: Data driven approach to approximate the modes and eigenvalues of the Koopman operator without numerically implementing a laplace transform

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- How do we define *best?*

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- Then $P_r U|_{\mathcal{K}_r} : \mathcal{K}_r \to \mathcal{K}_r$ is a finite dimensional linear operator

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- Restricting our attention on a fixed observable F and a Krylov subspace, the problem of finding eigenvalues and Koopman modes is reduced to finding eigenvalues and eigenvectors for matrix A_r

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- The top r eigenvalues of H_r approximate that of A_r

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- Think of them as point evaluations of the $\{U^k F\}$ basis for the Krylov subspace $\mathcal{K}_r$ at point $p \in M$

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- With $\mathbf{e} = (0, \ldots, 0, 1)^T \in \mathbb{C}^m$ and

$$A_r = \begin{bmatrix} 0 & 0 & \ldots & 0 & c_0 \\ 1 & 0 & \ldots & 0 & c_1 \\ 0 & 1 & \ldots & 0 & c_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & c_{r-1} \end{bmatrix}$$

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- A_r is the companion matrix ; a representation of $P_r U$ in the $\{U^k F\}_{k=0}^{r-1}$ basis

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- Define $E := K_r V^{-1}$, to get $UE = E\Lambda + \eta_r \mathbf{e}^T V^{-1}$

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- The version described is numerically ill-conditioned (columns of K_r can become linearly dependent)

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- The DMD modes and eigenvalues are eigenvalues and eigenvectors of A

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- The DMD mode corresponding to λ is given as:

$$\Phi = \frac{1}{\lambda} Y V \Sigma^{-1} w$$

Kernel Trick and Learning the Subspace

- Kernels
- Neural Networks