Linearization theorems, Koopman operator and its application

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Introduction

- Linear and nonlinear dynamics
- Local and global linearization

2 linearization in large

- Extensions of Hartman's theorem
- Examples
- The Koopman operator
 - Its introduction
 - Koopman operator and partition of the phase space

Applications

- The standard map
- Application to fluid dynamics



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Linear and nonlinear dynamics Local and global linearization

Complex systems-its characterization

• Hierarchical Structure

Many agents interconnected in a complex manner, resulting in a multi-scale, highly heterogeneous system.

• Self-organized dynamics

Nonlinear, non-equilibrium dynamics leads to the emergent behavior, which is non-reducible and unpredictable from single agent behavior.

Adaptability

Robust while flexible, evolvable.

• Uncertainties

The determination of parameters and relations are hard.



Introduction

Linear and nonlinear dynamics

The internetiverse





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Linear and nonlinear dynamics

Turbulence





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Structure of macromolecules





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Cell regulatory networks



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Linearization theorems, Koopman operator and its application

Linear and nonlinear dynamics Local and global linearization

Nonlinear dynamics: triumph and challenge

- Triumph of theory of nonlinear dynamical systems Local: linear stability analysis, bifurcation theory, normal form theory, ...
 - Global: Asymptotic analysis, topological methods, symbolic dynamics,...
- Troubles when treating complex systems
 - (1) Huge number of interacting agents (high-dimensional)
 - (2) Heterogeneity in spatiotemporal scales (numerical challenge)
 - (3) Hierarchical structure and great many dynamic modes
 - (4) Lack of exact mathematical description
 - (5) Uncertainty in data or parameters (noise or ignorance)



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Linear and nonlinear dynamics Local and global linearization

Linear systems and their solution

• General form: $\dot{\mathbf{x}} = A\mathbf{x}$ with

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & \cdots \\ \cdots & \cdots & \cdots & a_{n,1} \\ a_{n,1} & a_{n,2} & \cdots & a_{n,n} \end{pmatrix} \text{ and } \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

- Idea: separate solutions into independent modes by assuming $\mathbf{x}(t) = e^{\lambda t} \mathbf{v}$.
- We then obtain an **eigenvalue equation**

$$A\mathbf{v} = \lambda \mathbf{v}$$
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Linearization of nonlinear systems



- Hartman's theorem and Poincaré-Siegel theorem.
- Global linearization: weak nonlinearity or symmetry by lie group theory.



Linear and nonlinear dynamics Local and global linearization

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Extensions of Hartman's theorem $\operatorname{Examples}$

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Extensions of Hartman's theorem $\operatorname{Examples}$

Linearization in large

• Extension of Hartman's theorem for differential flows.

- The theorem can be extended to diffeomorphic mappings or flows with periodic driving.
- Linearization around an attractive or repulsive periodic orbit.
- How to treat saddles?



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Two examples

• Consider the 1-d equation $\dot{x} = x - x^3$. The transformation

$$x = b(y) = \frac{y}{\sqrt{1+y^2}}$$

results in $\dot{y} = y$, valid for $x \in [-1, 1]$.

• Consider the 2-d system $\dot{z_1} = 2z_1$, $\dot{z_2} = 4z_2 + z_1^2$. The transformation

$$z_1 = y_1, z_2 = y_2 + t(y_1, y_2)y_1^2$$

where $t(y_1, y_2) = \frac{1}{4} \ln y_1^2$ results in

 $\dot{y}_1 = 2y_1, \dot{y}_2 = 4y_2.$

[Y. Lan and I. Mezic, Physica D. 242, 42(2013)]



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Remarks on the linearization theorem

- According to Morse theory, the whole phase space of a hyperbolic system can be viewed as a gradient(-like) system modulo the minimal invariant sets. The phase space is a juxtaposition of linearizable patches.
- Problems:
 - (1) Hard to identify the linearization transformation.
 - (2) Works only for equilibria and periodic orbits.
 - (3) Hard to treat systems with conservation laws, e.g. Hamiltonian systems.



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Koopman operator, a way out?

• Statistical treatment of dynamical systems: Evolution of densities: the Perron-Frobenius Operator in analogy with the Schrödinger picture;

Evolution of observables: the Koopman operator in analogy with the Heisenberg picture.

- For a map $x_{n+1} = f(x_n)$ and a function g(x), the Koopman operator $U \circ g(x) = g(f(x))$
- For a flow $\phi(x,t)$ and a function g(x), a semigroup of Koopman operators could be defined as $U_t \circ g(x) = g(\phi(x,t)).$



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Eigenvalues and eigenmodes

- It is linear so its eigenvalues and eigenmodes are interesting objects.
- Examples:

(1) For a 1-d linear map $x_{n+1} = \lambda x_n$ and the observable $g(x) = x^m$,

$$U \circ g(x) = (\lambda x)^m = \lambda^m x^m = \lambda^m g(x).$$

• In fact, for C^1 observables, the most general form of the eigenfunction with eigenvalue λ^a is

$$g(x) = x^a \hat{g}(\ln x) \,,$$

where $\hat{g}(\cdot)$ is periodic with period $\ln \lambda$.



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Eigenvalues and Eigenmodes (continued)

• Examples:

(2) For a 1-d equation $\dot{x} = \lambda x$ and observable $g(x) = x^n$

$$U_t \circ g(x) = (xe^{\lambda t})^n = e^{n\lambda t}x^n = e^{n\lambda t}g(x)$$

- In fact, for C^1 observables, it can be proven that the general form of the eigenfunction is just as above.
- Extension to multi-dimensional linear systems and time periodic linear systems with a hyperbolic fixed point.

[Y. Lan and I. Meziź, Spectrum of the Koopman operator based on linearization, in preparation]



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The Koopman operator

Its introduction

Nontrivial examples

• Note that a(x) in the Hartman-Grobman's theorem satisfies

$$U_t a(x) = a \circ \phi(x, t) = e^{At} a(x)$$

• Suppose

$$V^{-1}a \circ \phi(x,t) = V^{-1}e^{At}a(x),$$

$$k \circ \phi(x_0, t) = e^{\Lambda t} k(x_0)$$



Its introduction Koopman operator and partition of the phase space

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$$U_t a(x) = a \circ \phi(x, t) = e^{At} a(x)$$

• Suppose

$$V^{-1}AV = \Lambda \,,$$

then we get

$$V^{-1}a \circ \phi(x,t) = V^{-1}e^{At}a(x),$$

and so $k = V^{-1}a$ satisfies

$$k \circ \phi(x_0, t) = e^{\Lambda t} k(x_0)$$

i.e. each component function of k is an eigenfunction of U_t .



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Construction of eigenmodes along trajectories

• For the map $x_{n+1} = T(x_n)$ and function g(x), consider

$$g^*(x) = \lim_{n \to \infty} \frac{1}{n} \sum_{j=0}^{n-1} g(T^j x),$$

which is an eigenfunction of the Koopman operator with eigenvalue 1.

• Furthermore, the construction

$$g^{\omega}(x) = \lim_{n \to \infty} \frac{1}{n} \sum_{j=0}^{n-1} e^{i2\pi j\omega} g(T^j x)$$

defines an eigenfunction of the Koopman operator with eigenvalue $e^{-i2\pi\omega}$.



The Koopman operator

Koopman operator and partition of the phase space

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Its introduction Koopman operator and partition of the phase space

Connection with Liouville operator

• In a Hamiltonian system with H(p,q), the Liouville operator L may be defined as

$$L \circ f(x) = -i \sum_{j} \left[\frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right],$$

which could be written with the Poisson bracket $L \circ f(x) = -i[f, H].$

- \bullet It is related to Koopman operator by the exponentiation $U_t = \exp(itL) \,. \label{eq:Ut}$
- On a transitive invariant set, Koopman operator is unitary, *i.e.*

$$U_t g(x) = e^{it\alpha} g(x) = e^{i(t\alpha + \arg(g))} |g(x)|.$$

|g(x)| is invariant and the phase increases linearly. Hence, they constitute the action-angle variable.



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Spectral decomposition of evolution equations

- For an evolution equation in an infinite-dimensional Hilbert space $v(x)^{n+1} = N(v(x)^n, p)$ and if the attractor M is of finite dimension with the evolution $m^{n+1} = T(m^n)$. For an observable g(x, m), we have $Ug(x, m) = U_s g(x, m) + U_r g(x, m)$ $= g^*(x) + \sum_{j=1}^k \lambda_j f_j(m) g_j(x) + \int_0^1 e^{i2\pi\alpha} dE(\alpha) g(x, m)$.
- U_s : the singular part of the operator corresponding to the discrete part of the spectrum, viewed as a deterministic part.

 U_r : the regular part of the operator corresponding to the continuous part of the spectrum, modeled as a stochastic process.

[I. Mezic, Nonlinear Dynamics 41, 309(2005)], (B) (B)

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The standard map

• The Chirikov standard map is

 $x_1^* = x_1 + 2\pi\epsilon \sin(x_2)(mod2\pi)$

 $x_2^* = x_1^* + x_2(mod2\pi)$

• The embedding of dynamics into space of three observables.

[M. Budisic and I. Mezic, 48th IEEE Conference on Decision and Control]



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Organizing invariant set by diffusion map





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Fluid dynamics

• The Navier-Stokes equation

$$\mathbf{v}_t + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{v}$$

with $\nabla\cdot\mathbf{v}=0$ describes incompressible Newtonian fluids.

- With different Reynold's number $Re = Lv/\nu$, the system experience a series of bifurcation: laminar \rightarrow periodic \rightarrow turbulent
- Turbulence is a spatiotemporal chaos with enormous space-time structures and scales.
- Jet in cross flow: turbulent but with large eddies. Could we describe it with the Koopman operator approach?



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Jet in cross flow



[C. W. Rowley et al, J. Fluid Mech. 641, 115(2009)]



The Arnoldi algorithm

• Consider a linear dynamical system $x_{k+1} = Ax_k$ and construct the matrix

$$K = [x_0, x_1, \cdots, x_{m-1}] = [x_0, Ax_0, \cdots, A^{m-1}x_0].$$

If the *m*th iterate $x_m = Ax_{m-1} = \sum_{k=0}^{m-1} c_k x_k + r$, the we can write $AK \approx KC$, where

$$C = \begin{pmatrix} 0 & 0 & 0 & \cdots & c_0 \\ 1 & 0 & 0 & \cdots & c_1 \\ 0 & 1 & 0 & \cdots & c_2 \\ & \cdots & & & \cdots & \\ 0 & \cdots & 0 & 1 & c_0 \end{pmatrix}$$

• If $Ca = \lambda a$, then the value λ and the vector v = Ka are approximate eigenvalue and eigenvector of the original matrix A.



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• Consider a linear dynamical system $x_{k+1} = Ax_k$ and construct the matrix

$$K = [x_0, x_1, \cdots, x_{m-1}] = [x_0, Ax_0, \cdots, A^{m-1}x_0].$$

If the *m*th iterate $x_m = Ax_{m-1} = \sum_{k=0}^{m-1} c_k x_k + r$, the we can write $AK \approx KC$, where

$$C = \begin{pmatrix} 0 & 0 & 0 & \cdots & c_0 \\ 1 & 0 & 0 & \cdots & c_1 \\ 0 & 1 & 0 & \cdots & c_2 \\ & \cdots & & \cdots & & \\ 0 & \cdots & 0 & 1 & c_0 \end{pmatrix}$$

• If $Ca = \lambda a$, then the value λ and the vector v = Ka are approximate eigenvalue and eigenvector of the original matrix A.



The standard map Application to fluid dynamics

Two structure functions





- Linearization is possible in the basin of attraction of a hyperbolic set.
- Koopman operator provides a way to identify the linearization transformation.
- On the minimal invariant set, the spectrum of the Koopman operator is on the unit circle.
- The eigenmodes could be constructed through numerical computation, revealing the most important dynamics.
- Generalizations and challenges:
 - (1) Can deal with stochastic systems.
 - (2) How to deal with uncertainty in complex systems.
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