MT1: Dynamic Mode Decompositions and Koopman Analysis

Introduction to Koopman Analysis

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with J. Nathan Kutz (U Wash), M. Hemati (U Minn)

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SIAM DS19 Snowbird, 2019

- **Koopman operator**:
  exact linear representation of (nonlinear) dynamics
- Koopman **eigenfunctions**:
  generalize Lyapunov functions, isochrons,…
- Koopman **modes**:
  in spirit, analogous to normal modes for linear PDEs
- data-driven (model-free) calculation enabled by (a family of) **Dynamic Mode Decomposition (DMD)** algorithm(s) (see J. N. Kutz's talk)
- can be **applied to** reduced-order modeling, global linearization, system ID, sensitivity, control... (see M. Hemati's talk)

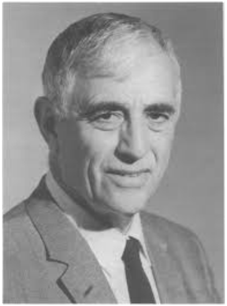
Related sessions

- MS48 Koopman Operator Techniques in Dynamical Systems: Theory
- MS61 Advanced Data-Driven Techniques and Numerical Methods in Koopman Operator Theory - Part I of II
- MS74 Advanced Data-Driven Techniques and Numerical Methods in Koopman Operator Theory - Part II of II
- MS86 Applications of Koopman Operator Theory in Dynamical Systems: From Fluids, through Machine Learning to Energy - Part I of II
- CP10 Data and Koopman Analysis
- MS97 Applications of Koopman Operator Theory in Dynamical Systems: From Fluids, through Machine Learning to Energy - Part II of II
- MS147 Control Techniques based on Koopman Operator Theory - Part I of II
- MS160 Control Techniques based on Koopman Operator Theory - Part II of II
- MS164 Theory and Application of Koopman Operator Methods in Molecular Simulation
- CP36 Koopman Analysis
- …and a whole bunch of sessions on reduced-order models, data-driven nonlinear analysis, etc.

Goals of this talk:

- explain the basics
- give some intuition
- point to active research areas

History and Present



Bernard Koopman

Vol. 17, 1931 *MATHEMATICS: B. O. KOOPMAN* 315

HAMILTONIAN SYSTEMS AND TRANSFORMATIONS IN HILBERT SPACE

By B. O. Koopman

Department of Mathematics, Columbia University

George Birkhoff

Vol. 18, 1932 *MATHEMATICS: BIRKHOFF AND KOOPMAN* 279

RECENT CONTRIBUTIONS TO THE ERGODIC THEORY

By G. D. Birkhoff and B. O. Koopman

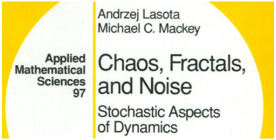
Department of Mathematics, Harvard University

John von Neumann

ZUR OPERATORENMETHODE IN DER KLASSISCHEN MECHANIK[1].

Von J. v. Neumann, Princeton.

Although Koopmanism (then: *Koopmania*) was present in 90s monographs…



It's the development of data-driven algorithms…

Nonlinear Dynamics (2005) 41: 309–325 © Springer 2005

Spectral Properties of Dynamical Systems, Model Reduction and Decompositions

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(Received: 25 May 2004; accepted: 15 June 2004)

J. Fluid Mech. (2010), *vol.* 656, *pp.* 5–28. © Cambridge University Press 2010 5
doi:10.1017/S0022112010001217

Dynamic mode decomposition of numerical and experimental data

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(Received 20 May 2009; revised 7 March 2010; accepted 7 March 2010; first published online 1 July 2010)

J. Fluid Mech. (2009), *vol.* 641, *pp.* 115–127. © Cambridge University Press 2009 115
doi:10.1017/S0022112009992059

Spectral analysis of nonlinear flows

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(Received 15 May 2009; revised 8 September 2009; accepted 9 September 2009; first published online 18 November 2009)

…that brought us here.

Introduction

Dynamics of states

Linear system $\underline{z}(t) = \begin{bmatrix} x(t) \\ y(t) \end{bmatrix}$

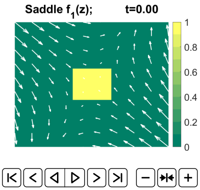
$$\dot{\underline{z}}(t) = \mathbf{A}\underline{z}(t), \underline{z}(0) = \underline{z}_0 \qquad \text{(ODE)}$$

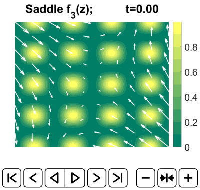
$$\underline{z}(t) = \underbrace{\exp\left(\mathbf{A}t\right)\underline{z}_0}_{\Phi^t(z_0)} \qquad \text{(Flow map)}$$

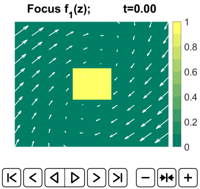
Dynamics of measurements

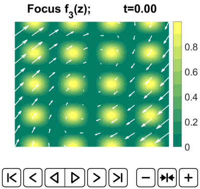
Measurement (*observable*) $h : \mathbb{R}^2 \to \mathbb{R}$, evolves along a trajectory according to:

$$h_t(\underline{z}_0) = h(\underline{z}(t)) = h(\Phi^t(\underline{z}_0))$$









KOOPMAN OPERATOR EVOLVES MEASUREMENTS.

General nonlinear systems:

$$\dot{\underline{z}}(t) = f(\underline{z}(t)), \underline{z}(0) = \underline{z}_0 \qquad \text{(ODE)}$$

$$\underline{z}(t) = \Phi^t(z_0) \qquad \text{(Flow map)}$$

Measurement evolution:

Koopman operator

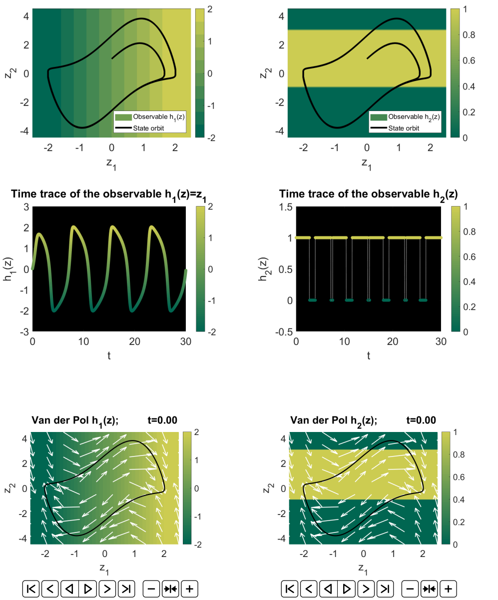
$$\mathbb{K}^t : \mathrm{Fun} \to \mathrm{Fun}$$

$$[\mathbb{K}^t h](\underline{z}) = h(\Phi^t(\underline{z}))$$

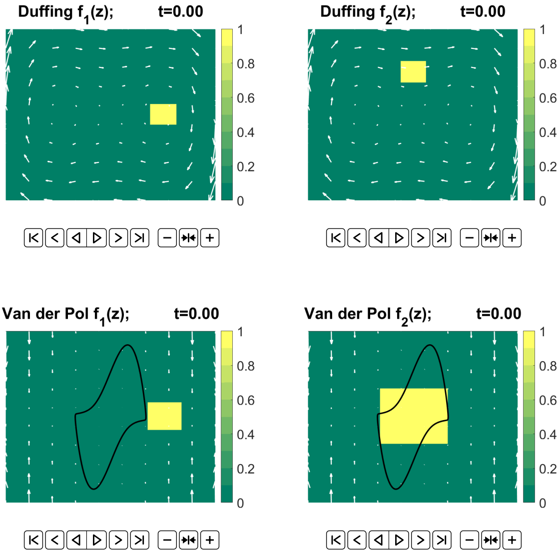
$$\mathbb{K}^t h = h \circ \Phi^t$$

a.k.a. pull-back by evolution/flow

a.k.a. composition operator



Starting to compute with Koopman…



Recipe:

- Seed a grid of initial conditions z_k
- Compute a trajectory from each point $z_k \rightsquigarrow z_k(t)$
- Evaluate the (scalar) function $f(z_k(t)) =: \mathbb{K}^t f(z_k)$ at final point
- Plot color field $\mathbb{R}^2 \mapsto \mathbb{R}$

$$z_k \mapsto [\mathbb{K}^t f](z_k)$$

Koopman operator is linear.

Koopman operator $\mathbb{K} : \text{Fun} \to \text{Fun}$ is
linear by construction

$$\underbrace{(\alpha f + \beta g) \circ \Phi^t}_{\mathbb{K}^t(\alpha f + \beta g)} = \alpha \underbrace{f \circ \Phi^t}_{\mathbb{K}^t f} + \beta \underbrace{g \circ \Phi^t}_{\mathbb{K}^t g}$$

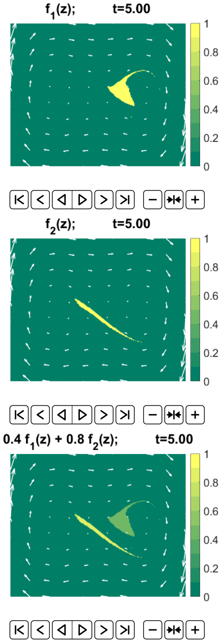
No magic: this is **not linearity in state** variables

$$\mathbb{K} f(\alpha z + \beta w) \neq \mathbb{K} f(\alpha z) + \mathbb{K} f(\beta w)$$

Trade-off

Flow map Φ^t	Koopman o. $\mathbb{K}^t$
Non-linear	Linear
Finite dim.	∞-dim.

No trade off if Φ^t is ∞-dimensional itself!



Spectral theory

- ergodic dynamics + L_2 space of observables = $\mathbb{K}$ is unitary
- in this case, Koopman op. is adjoint to the Perron–Frobenius transfer operator

Spectral Decomposition of the Koopman Operator

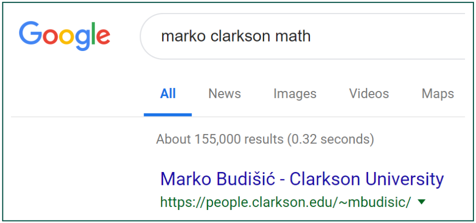
$$\mathbb{K}^n f = \int_{-\pi}^{\pi} e^{in\omega} d[\mathbb{E}(\omega) f] = \underbrace{\sum_k e^{in\omega_k} \mathbb{P}_k f}_{\text{atomic}} + \underbrace{\int_{-\pi}^{\pi} e^{in\omega} d[\mathbb{E}_c(\omega) f]}_{\text{continuous}}.$$

- **atomic spectrum $\rightarrow$ eigenvalues $\rightarrow$ (quasi)regular dynamics**
- a.c. spectrum $\rightarrow$ density function $\rightarrow$ mixing dynamics
- s.c. spectrum $\rightarrow$ fractal $\rightarrow$ “anomalous transport”

What is applied Koopman analysis?

- approximation of the Koopman operator from data
- computational spectral analysis
- interpretation and application of results

The PDF of this talk online (soon) on my website:



Koopman eigenfunctions

EIGENFUNCTIONS FOR LINEAR DYNAMICS (SADDLE)

$$\dot{z}(t) = \mathbf{A}z(t), z(0) = z_0$$
$$z(t) = \exp\left(\mathbf{A}t\right) z_0$$

Given left eigenvector at $\lambda \in \mathbb{R}$:

$$v^* \mathbf{A} = \lambda v^*, \quad v^* \exp(\mathbf{A}t) = e^{\lambda t} v^*$$

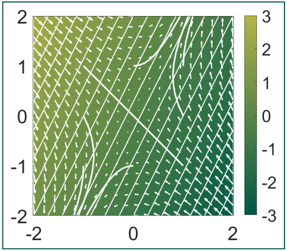
Functions

$$h(z) = v^* z$$

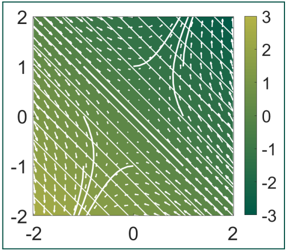
are **eigenfunctions** at $e^{\sigma t}$

$$h(z) = (v^* z)$$
$$\mathbb{K}^t\, h(z) = v^* e^{\mathbf{A}t} z = e^{\lambda t} \underbrace{v^* z}_{h(z)}$$

$h(z) = (v_1^* z)$



$h(z) = (v_2^* z)$



Structure of level sets stays constant in time. Values grow/decay according to eigenvalues.

Eigenfunctions for linear dynamics (focus)

$$\dot{z}(t) = \mathbf{A}z(t), z(0) = z_0$$
$$z(t) = \exp(\mathbf{A}t)\, z_0$$

Given left e.-vectors $v_+, v_- = \bar{v}$ at $\sigma \pm i\omega$:

$$v_\pm^* \mathbf{A} = \lambda v_\pm^*, \quad v_\pm^* \exp(\mathbf{A}t) = e^{\sigma t \pm i\omega t} v^*$$

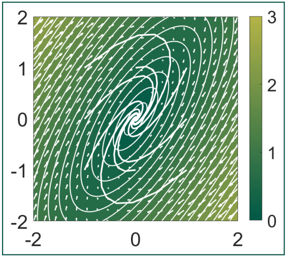
Functions

$$h(z) = (v^* z)(\bar{v}^* z)$$

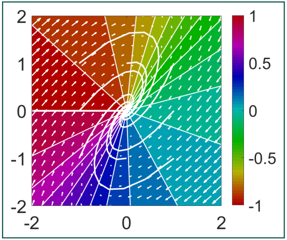
are **eigenfunctions** at $e^{\sigma t}$

$$h(z) = (v^* z)(\bar{v}^* z) = |v^* z|^2$$
$$\mathbb{K}^t\, h(z) = (v^* e^{\mathbf{A}t} z)(\bar{v}^* e^{\mathbf{A}t} z) = e^{\sigma t} \underbrace{(v^* z)(\bar{v}^* z)}_{h(z)}$$

$h(z) = (v^* z)(\bar{v}^* z)$



$h(z) = \angle(v^* z)$



Level sets correspond to a **Lyapunov function** $|v^* z|^2$ and **isochrons** $\angle(v^* z)$.

How to calculate eigenfunctions

Trajectory averages $z_{n+1} = \Phi(z_n)$ project **any** observable onto an eigenfunction:

$$h_\omega(z_0) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=0}^{N-1} \underbrace{\lambda^n}_{\text{E-value.}} \overbrace{h(z_n)}^{[\mathbb{K}^n h](z_0)}$$

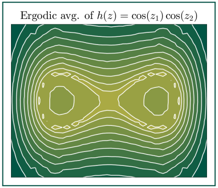
- **Ergodic average** – $\lambda = 0$ – invariant functions
- **Harmonic average** – $\lambda = e^{i\omega}$ – (quasi)periodic functions

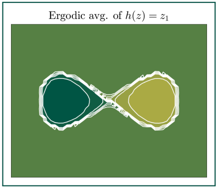
Recipe for eigenfunctions

1. Seed a grid of initial conditions z_k.
2. Simulate (long) trajectories $z_k \rightsquigarrow z_k(t)$.
3. Choose an observable and a frequency ω.
4. Compute the harmonic average and visualize $z_k \mapsto h_\omega(z_k)$.
   (If you choose a non-eigenvalue $e^{i\omega}$ you'll get $h_\omega \equiv 0$.)

Ergodic Average (double-well oscillator)

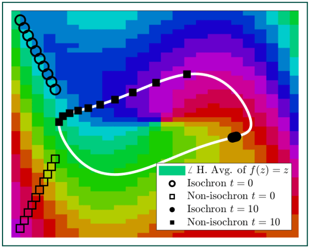
- Ergodic averages of observables are conserved quantities.
- Level sets of ergodic averages are invariant sets.

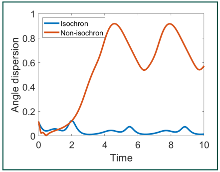




Harmonic Average (van der Pol oscillator)

- Angle of harmonic average of $h(z) = z$ at frequency of limit cycle.
- Level curves are isochrons.





Active Research Topics

- spectral theory for transient (non-steady-state) dynamical systems
- global stability and global linearization based on Koopman eigenfunctions
- control and system identification based on Koopman spectral analysis
- numerical methods for approximations and analysis of Koopman operator
- investigations into the spectral measure and non-atomic Koopman spectrum
- rigorous extensions of the Koopman theory for PDEs and SPDEs
- Koopman theory in reproducing kernel Hilbert spaces

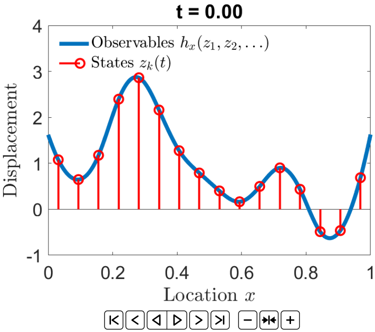
IPAM Operator Theoretic Methods in Dynamic Data Analysis and Control, Feb 2019, (link with videos)

Speakers: Nelida Črnjarić-Žic (University of Rijeka) Zlatko Drmač (University of Zagreb) Maria Fonoberova (AIMdyn) Gary Froyland (University of New South Wales) Dimitris Giannakis (New York University, Courant Institute of Mathematical Sciences) Didier Henrion (Centre National de la Recherche Scientifique (CNRS), Laboratoire d'Analyse et d'Architecture des Systemes (LAAS)) Maria Infusino (Universität Konstanz) Oliver Junge (Technical University of Munich) Milan Korda (Centre National de la Recherche Scientifique (CNRS)) J. Nathan Kutz (University of Washington, Applied Mathematics) Jean Lasserre (Université de Toulouse III (Paul Sabatier), LAAS-CNRS) Yuri Latushkin (University of Missouri-Columbia) Senka Maćešić (University of Rijeka) Krithika Manohar (California Institute of Technology, Computing and Mathematical Sciences) Alexandre Mauroy (Université de Namur) Igor Mezic (University of California, Santa Barbara (UCSB), Mechanical Engineering) Ryan Mohr (University of California, Santa Barbara (UCSB)) Nader Motee (Lehigh University, Mechanical Engineering and Mechanics) Hiroya Nakao (Tokyo Institute of Technology) Frank Noe (Freie Universität Berlin) Mihai Putinar (University of California, Santa Barbara (UCSB), Mathematics) Peter Schmid (Imperial College, Mathematics) Amit Surana (United Technologies Research Center) Umesh Vaidya (Iowa State University, Mechanical Engineering) Irène Waldspurger (Université de Paris IX (Paris-Dauphine)) Tillmann Weisser (Los Alamos National Laboratory) Enoch Yeung (University of California, Santa Barbara (UCSB))

Koopman modes

Linear PDEs: Normal mode analysis

- **States**: Simulated 16 linear oscillators
- **Observables**: Displacement between them (polynomial interpolation)
- Observables are **indexed** by *x* – there is a continuum of them.



- Interpretation: discretized wave equation.
- **Normal modes:** *x*−spatial profiles oscillating at isolated frequencies (standing waves).
- **Modes do not depend on state representation** (could have used spectral instead of FD solver...)

If $f \in \mathrm{span}(\text{eigenfunctions})$ we can **decompose it into eigenfunctions**.

$$f(z) = \sum_k \underbrace{m_k}_{\text{Coefficients}} \overbrace{h_k(z)}^{\text{E-fun.}} \qquad \text{(Observable)}$$

$$\mathbb{K}^t f(z) = \sum_k \underbrace{m_k}_{\text{Coefficients}} \overbrace{\lambda_k^t}^{\text{E-val.}} h_k(z) \qquad \text{(Evolution)}$$

Now, consider *many* observables $f_x(z)$ for $x \in S$

$$\mathbb{K}^t f_x(z) = \sum_k \underbrace{m_k(x)}_{\text{Koopman mode}} \lambda_k^t h_k(z)$$

Koopman mode $m_k(x)$

Demonstrates importance of eigenvalue λ_k across a measurements indexed by x.

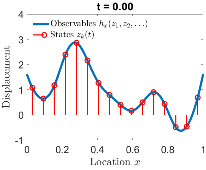
Normal mode analysis

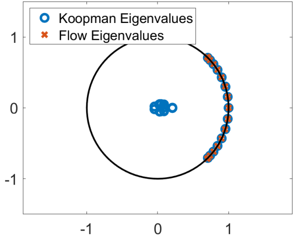
- model-dependent
- analytic
- works for select (non)linear systems

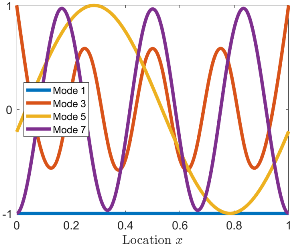
Koopman mode analysis

- model-free (data-driven)
- computational
- works for all (non)linear systems (they are after all just $\mathbb{K}$)

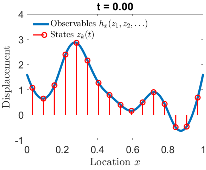
Koopman modes for linear vibrations

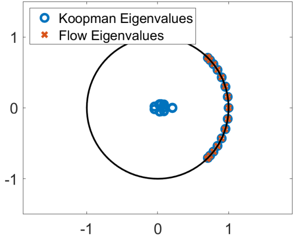


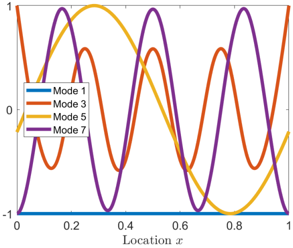




- Based on a single trajectory of dynamics
- Eigenvalues match the linear analysis
- Modes correctly capture the expected standing waves
- …but don't they look a bit funny at ends?
- Different trajectory (initial condition) could excite different modes







- Based on a single trajectory of dynamics

Computation (Dynamic Mode Decomposition)

Simulation data $\Rightarrow$ SVD $\Rightarrow$ EIG $\Rightarrow$ done.

…(much) more on this in the coming parts.

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modes

KOOPMAN MODE ANALYSIS EXTENDS NORMAL MODES TO NONLINEAR DYNAMICS.

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Spectral analysis of nonlinear flows

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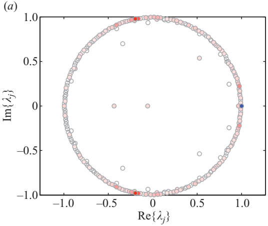
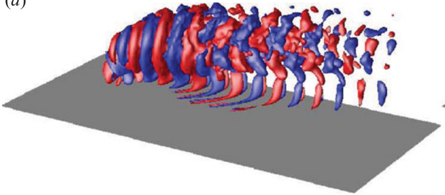
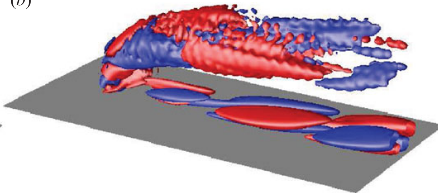


(*a*)



(*b*)



Where to start reading (a non-exhaustive list)

Papers:

AIP Chaos
An Interdisciplinary Journal of Nonlinear Science

Applied Koopmanism
Marko Budišić, Ryan Mohr, and Igor Mezić
Citation: Chaos: An Interdisciplinary Journal of Nonlinear Science **22**, 047510 (2012); doi: 10.1063/1.4772195

Annu. Rev. Fluid Mech. 2013. 45:357–78
First published online as a Review in Advance on October 5, 2012
The *Annual Review of Fluid Mechanics* is online at fluid.annualreviews.org
This article's doi: 10.1146/annurev-fluid-011212-140652
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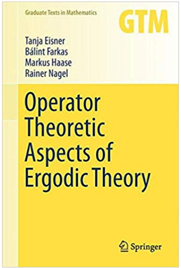
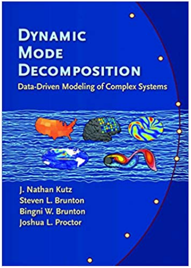
Analysis of Fluid Flows via Spectral Properties of the Koopman Operator
Igor Mezić
Department of Mechanical Engineering, University of California, Santa Barbara, California 93106; email: mezic@engineering.ucsb.edu

J Nonlinear Sci (2012) 22:887–915
DOI 10.1007/s00332-012-9130-9
Journal of Nonlinear Science

Variants of Dynamic Mode Decomposition: Boundary Condition, Koopman, and Fourier Analyses
Kevin K. Chen · Jonathan H. Tu · Clarence W. Rowley

Books:





Upcoming books:

- I. Mezić on spectral analysis of dynamical systems
- S. Brunton et al. on data-driven methods in dynamics

- **Koopman operator**:
  exact linear representation of (nonlinear) dynamics
- Koopman **eigenfunctions**:
  generalize Lyapunov functions, isochrons,...
- Koopman **modes**:
  in spirit, analogous to normal modes for linear PDEs
- data-driven (model-free) calculation enabled by (a family of) **Dynamic Mode Decomposition (DMD)** algorithm(s) (see J. N. Kutz's talk)
- can be **applied to** reduced-order modeling, global linearization, system ID, sensitivity, control... (see M. Hemati's talk)