Data-driven approximation of the Koopman operator

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Goals

- Determine approximations of Koopman eigenvalues/eigenfunctions/modes directly from data.
- Use these to try to learn features of dynamical systems
- Interested in high-dimensional systems (e.g., fluids)

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Outline

Dynamic Mode Decomposition and the Koopman operator

Definitions and a brief history

When does DMD approximate Koopman?

Example: two-dimensional map

Extended DMD

Collocation method to approximate Koopman

Example: basins of attraction in the Duffing equation

Dynamic Mode Decomposition: original definition

Dynamic Mode Decomposition (DMD) was originally defined by an algorithm[1]:

- Collect snapshots of data $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m$, equally spaced in time.
- Assume the data are linearly related:

$$\mathbf{x}_{k+1} = A\mathbf{x}_k$$

- Use an Arnoldi-like algorithm to approximate eigenvalues and eigenvectors of A (without ever determining A explicitly).

Hitch: Typically the dynamics are nonlinear, and the linear assumption does not hold.

[1] P.J. Schmid, APS 2008, JFM 2010

Dynamic Mode Decomposition: an alternative definition

Collect snapshots of data $\mathbf{x}_1, \ldots, \mathbf{x}_m$ and corresponding snapshots $\mathbf{x}_1^\#, \ldots, \mathbf{x}_m^\#$ one "timestep" later. (For a sequential time series, one takes $\mathbf{x}_k^\# = \mathbf{x}_{k+1}$.)

Definition (DMD)

Assemble the data into two matrices

$$X = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_m \end{bmatrix} \qquad X^\# = \begin{bmatrix} \mathbf{x}_1^\# & \mathbf{x}_2^\# & \cdots & \mathbf{x}_m^\# \end{bmatrix}.$$

The DMD modes are eigenvectors of

$$A = X^\# X^+,$$

where $+$ denotes the Moore-Penrose pseudoinverse.

- Under mild assumptions on the data (e.g., the measurements $\mathbf{x}_j$ are linearly independent), the data satisfy $\mathbf{x}_j^\# = A\mathbf{x}_j$.
- Thus, there still seems to be the assumption that the dynamics are linear. Yet it seems to give useful results for nonlinear problems...

J.H. Tu, C.W. Rowley, D.M. Luchtenburg, S.L. Brunton, and J.N. Kutz, *J. Computational Dynamics*, Dec 2014.

Koopman operator

Definition (Koopman, 1931)

Consider a discrete-time dynamical system on a measure space (Z, μ):

$$z \mapsto T(z).$$

The Koopman operator U acts on scalar functions f (e.g., $f \in L^2(Z)$), as

$$Uf(z) \triangleq f(T(z)).$$

- If T is measure preserving ($\mu(A) = \mu(T^{-1}A)$), then U is an isometry ($\|Uf\| = \|f\|$); if, in addition, T is invertible, then U is unitary.
- Suppose U has an eigenfunction φ, with $U\varphi = \lambda\varphi$, and let $y(k) = \varphi(z(k))$. Then

  $$y(k+1) = \varphi(z(k+1)) = U\varphi(z(k)) = \lambda\varphi(z(k)) = \lambda y(k),$$

  so y evolves according to linear dynamics.
- If U has enough eigenfunctions so that we can reconstruct the state z from the values of the eigenfunctions, then there is a coordinate change in which the system is linear.

Koopman and DMD

How is Koopman related to DMD?

- Consider a set of *observables* $\psi_j \in L^2(Z)$, $j = 1, \dots, n$, and let $\boldsymbol{\psi}$ denote the vector of observables.
- Consider a set of initial states $\{z_1, \dots, z_m\} \subset Z$, and let

$$\mathbf{x}_k = \boldsymbol{\psi}(z_k), \qquad \mathbf{x}_k^\# = \boldsymbol{\psi}(T(z_k)).$$

Define matrices X and $X^\#$ as before, and $A = X^\# X^+$.

Theorem (Koopman and DMD[3])

Let φ be an eigenfunction of U with eigenvalue λ, and suppose $\varphi \in \operatorname{span}\{\psi_j\}$, so that $\varphi(z) = \mathbf{w}^* \boldsymbol{\psi}(z)$ for some $\mathbf{w} \in \mathbb{C}^n$. If $\mathbf{w} \in \mathcal{R}(X)$, then $\mathbf{w}$ is a left eigenvector of A with eigenvalue λ: $\mathbf{w}^* A = \lambda \mathbf{w}^*$.

So Koopman eigenvalues are DMD eigenvalues, provided:

1. the set of observables is sufficiently large ($\varphi \in \operatorname{span}\{\psi_j\}$)
2. the data are sufficiently rich ($\mathbf{w} \in \mathcal{R}(X)$).

Furthermore, we can calculate the Koopman eigenfunctions from the *left* eigenvectors of the DMD matrix A, as $\varphi(z) = \mathbf{w}^* \boldsymbol{\psi}(z)$.

[3] Tu, Rowley, Luchtenburg, Brunton, and Kutz, *J. Comput. Dyn.*, 2014

Example: two-dimensional map

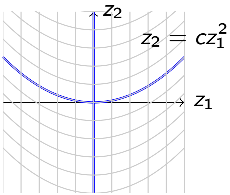
Caution

DMD with the "full-state observable" $\psi(\mathbf{z}) = \mathbf{z}$ typically does not work for a nonlinear system.

Consider the map

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \mapsto \begin{bmatrix} \lambda z_1 \\ \mu z_2 + (\lambda^2 - \mu) c z_1^2 \end{bmatrix}.$$

This system has an equilibrium at the origin, and invariant manifolds given by $z_1 = 0$ and $z_2 = c z_1^2$:



Koopman eigenvalues are λ, μ with eigenfunctions

$$\varphi_\lambda(\mathbf{z}) = z_1$$
$$\varphi_\mu(\mathbf{z}) = z_2 - c z_1^2.$$

In addition, φ_λ^k is an eigenfunction with eigenvalue λ^k, the product $\varphi_\lambda \varphi_\mu$ is an eigenfunction with eigenvalue $\lambda\mu$, etc.

DMD for two-dimensional map

Apply DMD to this example, with initial states $\mathbf{z}$ given by $(1,1),(5,5),(-1,1),(-5,5)$, with $\lambda = 0.9$, $\mu = 0.5$.

- Case 1: observable $\boldsymbol{\psi}(\mathbf{z}) = (z_1, z_2)$. If $c = 0$, so that the problem is linear, then DMD eigenvalues are 0.9 and 0.5: good!
  If $c = 1$, however, then the DMD eigenvalues are 0.9 and 2.002. These do not correspond to Koopman eigenvalues, and one might even presume the equilibrium is *unstable*!
- Case 2: observable $\boldsymbol{\psi}(\mathbf{z}) = (z_1, z_2, z_1^2)$. Now, the DMD eigenvalues are 0.9, 0.5, and $0.81 = 0.9^2$, which agree with Koopman eigenvalues.
- Case 3: observable $\boldsymbol{\psi}(\mathbf{z}) = (z_1, z_2, z_2^2)$. Now, the DMD eigenvalues are 0.9, 0.822, and 4.767. There is still a linear relationship between the snapshots ($\mathbf{x}_j^\# = A\mathbf{x}_j$), but the eigenvalues do not correspond to Koopman eigenvalues because the Koopman eigenfunction φ_μ is not in the span of the observables.

Outline

Approximating the Koopman operator

We can use spectral methods to approximate the Koopman operator. Consider the discrete-time dynamical system $z \mapsto T(z)$,

$$(Uf)(z) = f(T(z)) = (f \circ T)(z).$$

We expand a function f (and Uf) in terms of basis functions ψ_j:

$$f(z) = \sum_{j=1}^{N} a_j \psi_j(z), \qquad Uf(z) = \sum_{j=1}^{N} b_j \psi_j(z)$$

This approximation takes the form of a matrix that maps from $\mathbf{a}$ to $\mathbf{b}$.

Using a weighted residual method, $\mathbf{b} = \Psi^{+}\Psi^{\#}\mathbf{a}$, with

$$\Psi = \begin{bmatrix} \langle W_1, \psi_1 \rangle & \cdots & \langle W_1, \psi_N \rangle \\ \vdots & & \vdots \\ \langle W_M, \psi_1 \rangle & \cdots & \langle W_M, \psi_N \rangle \end{bmatrix}, \quad \Psi^{\#} = \begin{bmatrix} \langle W_1, \psi_1 \circ T \rangle & \cdots & \langle W_1, \psi_N \circ T \rangle \\ \vdots & & \vdots \\ \langle W_M, \psi_1 \circ T \rangle & \cdots & \langle W_M, \psi_N \circ T \rangle \end{bmatrix}$$

where $\langle W_i, \cdot \rangle$ denotes the inner product with the ith weight function.

A collocation method

Data rather than equations

All we have access to is a data set $\{\mathbf{x}_j, \mathbf{x}_j^{\#}\}_{j=1}^{M}$, with $\mathbf{x}_j = \boldsymbol{\psi}(z_j)$, $\mathbf{x}_j^{\#} = \boldsymbol{\psi}(Tz_j)$. The map T is unknown, and we cannot ask for more data.

- Choose $W_i(z) = \delta(z - z_i)$. Then

$$\boldsymbol{\Psi} = \begin{bmatrix} \psi_1(z_1) & \cdots & \psi_N(z_1) \\ \vdots & & \vdots \\ \psi_1(z_M) & \cdots & \psi_N(z_M) \end{bmatrix}, \quad \boldsymbol{\Psi}^{\#} = \begin{bmatrix} \psi_1(Tz_1) & \cdots & \psi_N(Tz_1) \\ \vdots & & \vdots \\ \psi_1(Tz_M) & \cdots & \psi_N(Tz_M) \end{bmatrix}$$

- The finite-dimensional approximation of U is

$$K \triangleq \boldsymbol{\Psi}^{+}\boldsymbol{\Psi}^{\#}.$$

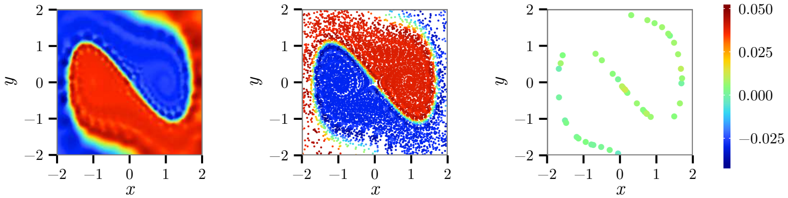
- The eigenvalues of K approximate the *eigenvalues* of U
- The eigenvectors approximate the *eigenfunctions* of U

Example: basins of attraction in the Duffing equation

- Consider the Duffing equation

$$\ddot{x} + \delta \dot{x} + x(x^2 - 1) = 0$$

- Compute EDMD (with $\delta = 0.5$):
  - Data: 10^3 trajectories with 11 samples each, sampling interval $\Delta t = 0.25$
  - Basis functions: 1000 radial basis functions (thin plate splines)
- $\lambda_0 = -10^{-14}$: corresponding eigenfunction is the constant function
- $\lambda_1 = -10^{-3}$: eigenfunction reveals basins of attraction



Dynamics in each basin

- $\lambda_2 = -0.237 + 1.387i$ (analytically $-0.250 + 1.392i$)