

MATH 4280

Lecture Notes 8: Data-driven dynamical systems

Dynamical systems

- We consider dynamical systems of the form

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t; \boldsymbol{\beta})$$

where \mathbf{x} is the state, \mathbf{f} is a given vector field and $\boldsymbol{\beta}$ is a set of parameters

- We will also consider simpler case of an autonomous system

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t))$$

where the right hand side has no time dependence or parameter

Discrete-time systems

- We also consider discrete-time systems

$$\mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k)$$

- Discrete-time dynamics may be induced from continuous-time dynamics, where $\mathbf{x}_k = \mathbf{x}(k\Delta t)$ is obtained the sampling in discrete times
- In this case, the discrete-time propagator $\mathbf{F}_{\Delta t}$ is parameterized by the time step Δt .
- For an arbitrary time, we define the flow map \mathbf{F}_t by

$$\mathbf{F}_t(\mathbf{x}(t_0)) = \mathbf{x}(t_0) + \int_{t_0}^{t_0+t} \mathbf{f}(\mathbf{x}(\tau)) d\tau$$

Linear dynamics

- We consider linear dynamics of the form

$$\frac{d}{dt}\mathbf{x} = \mathbf{A}\mathbf{x}$$

- The solution is given by

$$\mathbf{x}(t_0 + t) = e^{\mathbf{A}t}\mathbf{x}(t_0)$$

- The matrix A has the following spectral decomposition

$$\mathbf{A}\mathbf{T} = \mathbf{T}\mathbf{\Lambda}$$

- When the matrix A has distinct eigenvalues, we have $\mathbf{A} = \mathbf{T}\mathbf{\Lambda}\mathbf{T}^{-1}$ and

$$\mathbf{x}(t_0 + t) = \mathbf{T}e^{\mathbf{\Lambda}t}\mathbf{T}^{-1}\mathbf{x}(t_0)$$

where $\mathbf{\Lambda}$ is a diagonal matrix, columns of \mathbf{T} are eigenvectors

Goals

- Future state prediction: e.g. weather forecasting
- Design and optimization: tune the parameters of a system for improved performance
- Estimation and control: actively control a dynamical system through feedback
- Physical understanding: obtain insights of a system by analyzing the solutions

Challenges

- Nonlinearity: the main challenge
- Unknown dynamics: a lot of problems do not have known governing equations
- High dimensional dynamics: difficult to find patterns to uncover intrinsic coordinates which the dominant behavior evolves

Data-driven approaches

- Traditionally, physical systems are analyzed by making ideal approximations, resulting in simple models
- With increasing complex systems, the paradigm is shifting from classical approaches to data-driven methods to discover governing equations
- Determining the correct model is becoming more subjective, and there is a need for automated model discovery technique
- Thus, identifying unknown dynamics and learning intrinsic coordinates are the most pressing goals

Dynamic mode decomposition (DMD)

- DMD is used to identify **spatio-temporal coherent structures** in high dimensional data
- DMD is based on **proper orthogonal decomposition (POD)**
- DMD identifies the **best** linear dynamical system that advances high dimensional measurement forward in time
- DMD is **based purely on measurement data**

Basic ideas of DMD

- It is a data-driven approach
- First, collect a number of pairs of **snapshots** as they evolve in time
- We denote the snapshots as $\{(\mathbf{x}(t_k), \mathbf{x}(t'_k))\}_{k=1}^m$ where $t'_k = t_k + \Delta t$
- Here Δt is the time step, small enough to capture highest frequencies in the dynamics
- The snapshot is a state of the system sampled at a number of discretized locations

- The snapshots can be arranged into data matrices

reshape a snapshot into a 1D array

$$\mathbf{X} = \begin{bmatrix} \left. \begin{array}{c} | \\ \mathbf{x}(t_1) \\ | \end{array} \right. & \left. \begin{array}{c} | \\ \mathbf{x}(t_2) \\ | \end{array} \right. & \cdots & \left. \begin{array}{c} | \\ \mathbf{x}(t_m) \\ | \end{array} \right. \end{bmatrix}$$

$$\mathbf{X}' = \begin{bmatrix} \left. \begin{array}{c} | \\ \mathbf{x}(t'_1) \\ | \end{array} \right. & \left. \begin{array}{c} | \\ \mathbf{x}(t'_2) \\ | \end{array} \right. & \cdots & \left. \begin{array}{c} | \\ \mathbf{x}(t'_m) \\ | \end{array} \right. \end{bmatrix}$$

- Note, if we assume uniform sampling in time $t_k = k\Delta t$ and $t'_k = t_k + \Delta t = t_{k+1}$, we use the notation $\mathbf{x}_k = \mathbf{x}(k\Delta t)$

shifting the data entries by one

- The **DMD algorithm** seeks the best linear operator **A** that relates the two snapshot matrices in time

$$\mathbf{X}' \approx \mathbf{A}\mathbf{X}$$

- This best fit linear operator gives a linear dynamical system that advances snapshot measurements in time
- If we assume uniform sampling in time

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

- Mathematically, the linear operator is defined as

$$\mathbf{A} = \underset{\mathbf{A}}{\operatorname{argmin}} \|\mathbf{X}' - \mathbf{A}\mathbf{X}\|_F = \mathbf{X}'\mathbf{X}^\dagger$$

This is the .fit() step in the python script

- Note that **A** and its eigenvectors are expensive to compute due to large dimension

DMD algorithm

- Assume \mathbf{X} is $m \times n$, $m \ll n$
- Step 1: Compute the SVD of \mathbf{X}

$$\mathbf{X} \approx \tilde{\mathbf{U}} \tilde{\Sigma} \tilde{\mathbf{V}}^*$$

where $\tilde{\mathbf{U}} \in \mathbb{C}^{n \times r}$, $\tilde{\Sigma} \in \mathbb{C}^{r \times r}$ and $\tilde{\mathbf{V}} \in \mathbb{C}^{m \times r}$

- Here $r \leq m$ is the exact or approximate rank of the data matrix \mathbf{X}
- Recall that the columns of $\tilde{\mathbf{U}}$ are called **POD modes**

(= PCA modes)

- Step 2: Recall that the full matrix \mathbf{A} is computed as

$$\mathbf{A} = \mathbf{X}' \tilde{\mathbf{V}} \tilde{\mathbf{\Sigma}}^{-1} \tilde{\mathbf{U}}^*$$

- Note that we are interested in the leading r eigenvectors

- We project \mathbf{A} onto the POD modes (the space that spanned by $\tilde{\mathbf{U}}$)

$$\tilde{\mathbf{A}} = \tilde{\mathbf{U}}^* \mathbf{A} \tilde{\mathbf{U}} = \tilde{\mathbf{U}}^* \mathbf{X}' \tilde{\mathbf{V}} \tilde{\mathbf{\Sigma}}^{-1}$$

- Note that the reduced matrix $\tilde{\mathbf{A}}$ has the same nonzero eigenvalues as the full matrix \mathbf{A}
- The reduced matrix $\tilde{\mathbf{A}}$ defines a linear dynamic for POD modes

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

$$\mathbf{x}_{k+1} = \mathbf{A} \mathbf{x}_k, \quad \tilde{\mathbf{u}}^* \mathbf{x}_{k+1} = \tilde{\mathbf{u}}^* \mathbf{A} \mathbf{x}_k; \quad \tilde{\mathbf{x}}_{k+1} = \tilde{\mathbf{A}} \tilde{\mathbf{x}}_k$$

- The full state can be recovered by $\mathbf{x} = \tilde{\mathbf{U}} \tilde{\mathbf{x}}$

- Step 3: Perform the spectral decomposition of \tilde{A}

$$\tilde{A}\tilde{W} = \tilde{W}\Lambda$$

- Note that the diagonal matrix Λ contains the DMD eigenvalues, which are also eigenvalues of the full matrix A
- The columns of \tilde{W} are eigenvectors, which are linear combination of POD modes amplitudes

- Step 4: The high dimensional DMD modes Φ are reconstructed by

$$\Phi = X'\tilde{V}\tilde{\Sigma}^{-1}\tilde{W}$$

(Which has no explanation)

- Note that

$$A\Phi = (X'\tilde{V}\tilde{\Sigma}^{-1}\underbrace{\tilde{U}^*}_{\tilde{A}})(X'\tilde{V}\tilde{\Sigma}^{-1}\tilde{W})$$

$$= X'\tilde{V}\tilde{\Sigma}^{-1}\tilde{A}\tilde{W}$$

$$= X'\tilde{V}\tilde{\Sigma}^{-1}\tilde{W}\Lambda$$

$$= \Phi\Lambda.$$

DMD modes are eigenvectors

DMD expansion

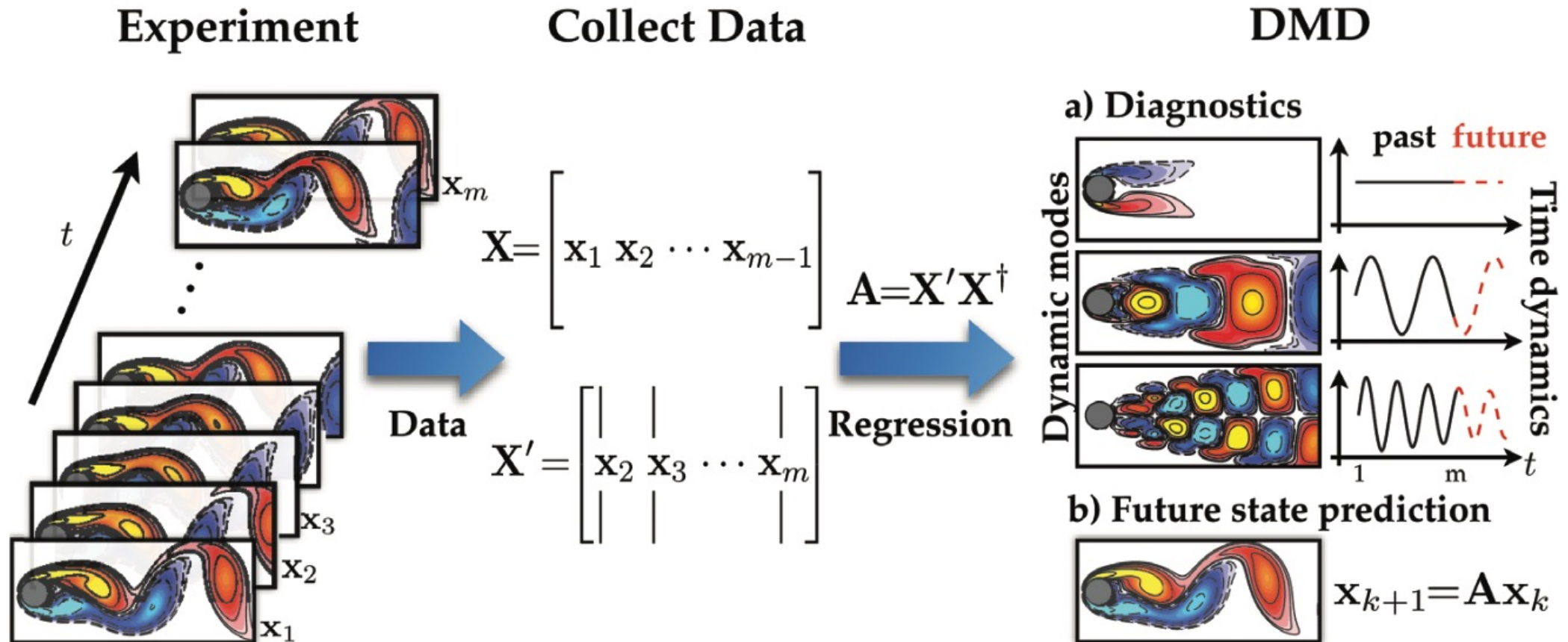
- We can use DMD modes to represent the state of the system

$$\mathbf{x}_k = \sum_{j=1}^r \phi_j \lambda_j^{k-1} b_j = \Phi \Lambda^{k-1} \mathbf{b}$$

- The vector \mathbf{b} is computed by $\mathbf{b} = \Phi^\dagger \mathbf{x}_1$
- A more convenient way to compute \mathbf{b}

$$\begin{aligned}\mathbf{x}_1 &= \Phi \mathbf{b} \\ \Rightarrow \tilde{\mathbf{U}} \tilde{\mathbf{x}}_1 &= \mathbf{X}' \tilde{\mathbf{V}} \tilde{\Sigma}^{-1} \mathbf{W} \mathbf{b} \\ \Rightarrow \tilde{\mathbf{x}}_1 &= \tilde{\mathbf{U}}^* \mathbf{X}' \tilde{\mathbf{V}} \tilde{\Sigma}^{-1} \mathbf{W} \mathbf{b} \\ \Rightarrow \tilde{\mathbf{x}}_1 &= \tilde{\mathbf{A}} \mathbf{W} \mathbf{b} \\ \Rightarrow \tilde{\mathbf{x}}_1 &= \mathbf{W} \Lambda \mathbf{b} \\ \Rightarrow \mathbf{b} &= (\mathbf{W} \Lambda)^{-1} \tilde{\mathbf{x}}_1.\end{aligned}$$

Overview of using DMD algorithm



Applications: fluid dynamics, neuroscience, video processing, etc

Sparse identification of nonlinear dynamics

- Discovering dynamical systems from data is a central challenge
- Sparse identification of nonlinear dynamics (SIND) considers

$$\frac{d}{dt}\mathbf{x} = \mathbf{f}(\mathbf{x})$$

- We seek the following approximation

$$\mathbf{f}(\mathbf{x}) \approx \sum_{k=1}^p \theta_k(\mathbf{x}) \xi_k = \Theta(\mathbf{x}) \boldsymbol{\xi}$$

with the fewest nonzero terms in $\boldsymbol{\xi}$

- We collect the following data for the states and their derivatives

$$\mathbf{X} = [\mathbf{x}(t_1) \quad \mathbf{x}(t_2) \quad \cdots \quad \mathbf{x}(t_m)]^T$$

$$\dot{\mathbf{X}} = [\dot{\mathbf{x}}(t_1) \quad \dot{\mathbf{x}}(t_2) \quad \cdots \quad \dot{\mathbf{x}}(t_m)]^T$$

- A library of candidate functions is used

$$\Theta(\mathbf{X}) = [1 \quad \mathbf{X} \quad \mathbf{X}^2 \quad \cdots \quad \mathbf{X}^d \quad \cdots \quad \sin(\mathbf{X}) \quad \cdots]$$

- The dynamical system is represented using data matrices

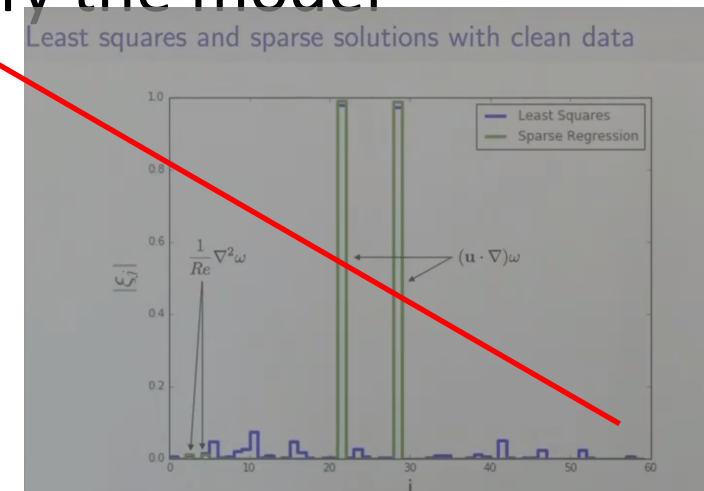
$$\dot{\mathbf{X}} = \Theta(\mathbf{X}) \Xi$$

- The following optimization problem is used to identify the model

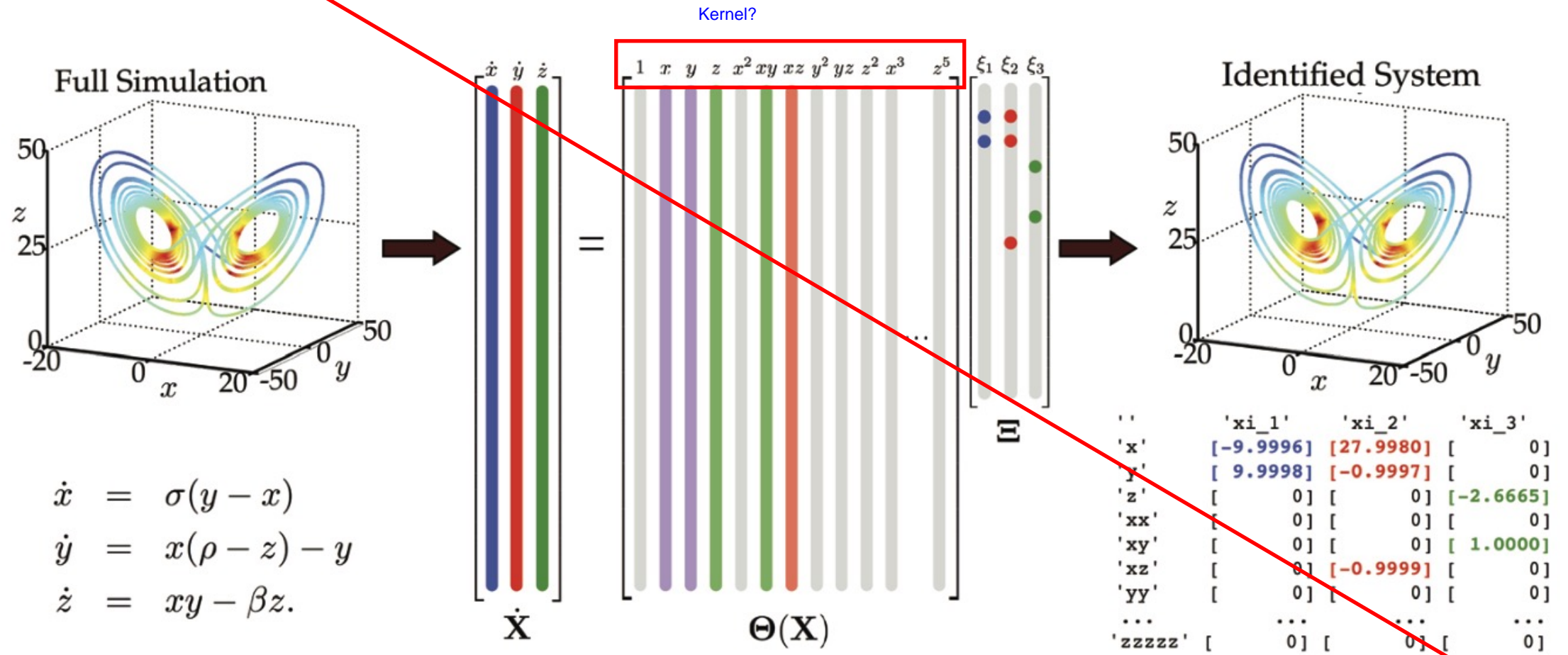
$$\xi_k = \operatorname{argmin}_{\xi'_k} \|\dot{\mathbf{X}}_k - \Theta(\mathbf{X}) \xi'_k\|_2 + \lambda \|\xi'_k\|_1$$

Bad approach: least squares - It is bad because ξ_i is almost surely dense.
Better approach: sparse regression

Green column: generated by sparse regression



Schematic of SIND



Discovering PDE

Data: if the data is not clean, we need to smoothen it.

- Let $\mathbf{r} \in \mathbb{C}^{mn}$ be space-time data, m is the number of time samples, and n is the number of spatial locations
- Additional input can be included in $\mathbf{Q} \in \mathbb{C}^{mn \times D}$ with D candidates of linear and nonlinear terms and partial derivatives is used, and it has the form

$$\Theta(\mathbf{r}, \mathbf{Q}) = [\mathbf{1} \quad \mathbf{r} \quad \mathbf{r}^2 \quad \dots \quad \mathbf{Q} \quad \dots \quad \mathbf{r}_x \quad \mathbf{r}\mathbf{r}_x \quad \dots]$$

- The PDE can be represented in this library by

$$\mathbf{r}_t = \Theta(\mathbf{r}, \mathbf{Q})\xi$$

- Then, we find the sparse vector ξ

Data + assumptions \Rightarrow linear system

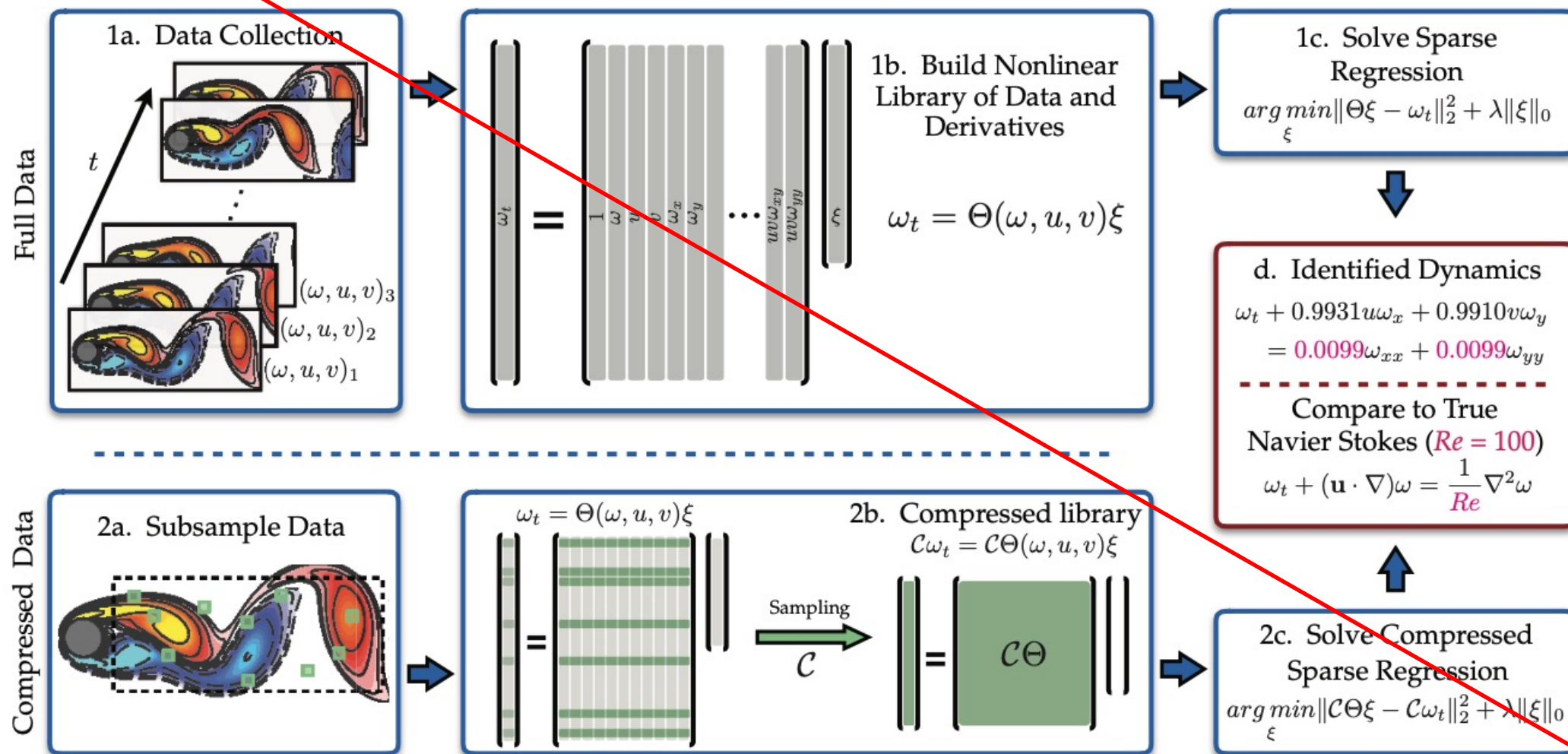
- 1 Collect data for discovery of PDE
 - \mathbf{U} is discretization of u across spatiotemporal domain
 - \mathbf{Q} is discretization of q on same domain

- 2 Numerically compute u_x, u_{xx}, \dots from \mathbf{U}

- 3 Create linear system to solve for ξ : $\mathbf{U}_t = \Theta(\mathbf{U}, \mathbf{Q})\xi$

$$\underbrace{\begin{pmatrix} u_t(x_1, t_1) \\ u_t(x_2, t_1) \\ \vdots \\ u_t(x_n, t_m) \end{pmatrix}}_{\mathbf{U}_t} = \underbrace{\begin{pmatrix} 1 & u(x_1, t_1) & u_x(x_1, t_1) & \dots & q^2 u^3 u_{xxx}(x_1, t_1) \\ 1 & u(x_2, t_1) & u_x(x_2, t_1) & \dots & q^2 u^3 u_{xxx}(x_2, t_1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & u(x_n, t_m) & u_x(x_n, t_m) & \dots & q^2 u^3 u_{xxx}(x_n, t_m) \end{pmatrix}}_{\Theta(\mathbf{U}, \mathbf{Q})} \xi$$

Schematic



Koopman operator

- Represent a **nonlinear dynamical system** in terms of an infinite dimensional **linear operator**
- This **Koopman operator** is linear, and its spectral decomposition completely characterizes the nonlinear dynamics
- Obtaining **finite dimensional approximation** of the Koopman operator is the focus of research

Linear matrix that advances measurements forward in time

Mathematical formulation

g could be any measurements of x in this Herbert space

- We let $g: M \rightarrow \mathbb{R}$ be a real-valued measurement function
- The Koopman operator \mathcal{K}_t is an infinite dimensional linear operator acting on measurement functions defined by

$$\mathcal{K}_t g = g \circ \mathbf{F}_t$$

(\mathbf{F}_t we considered before)

- For discrete time system, we have

$$\mathcal{K}_{\Delta t} g(\mathbf{x}_k) = g(\mathbf{F}_{\Delta t}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1})$$

from previous properties
we could have many choices of g

- Thus, the Koopman operator advances the observation of a state

$$g(\mathbf{x}_{k+1}) = \mathcal{K}_{\Delta t} g(\mathbf{x}_k)$$

- For smooth continuous time dynamical system, we can define the following Koopman dynamical system

$$\frac{d}{dt}g = \mathcal{K}g.$$

- The operator \mathcal{K} is defined as

$$\mathcal{K}g = \lim_{t \rightarrow 0} \frac{\mathcal{K}_t g - g}{t} = \lim_{t \rightarrow 0} \frac{g \circ \mathbf{F}_t - g}{t}$$

Koopman eigenfunctions

- Identify key measurement functions, that evolves linearly

- Discrete-time Koopman eigenfunctions are given by

$$\varphi(\mathbf{x}_{k+1}) = \mathcal{K}_{\Delta t} \varphi(\mathbf{x}_k) = \lambda \varphi(\mathbf{x}_k)$$

- Continuous-time Koopman eigenfunctions are given by

$$\frac{d}{dt} \varphi(\mathbf{x}) = \mathcal{K} \varphi(\mathbf{x}) = \lambda \varphi(\mathbf{x})$$

- Taking derivatives, we have

$$\frac{d}{dt} \varphi(\mathbf{x}) = \nabla \varphi(\mathbf{x}) \cdot \dot{\mathbf{x}} = \nabla \varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x})$$

- So, we obtain a PDE for the eigenfunctions

$$\nabla \varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = \lambda \varphi(\mathbf{x})$$

- We let $g: M \rightarrow \mathbb{R}$ be a real-valued measurement function
- The Koopman operator \mathcal{K}_t is an infinite dimensional linear operator acting on measurement functions defined by

- For discrete time system, we have

$$\mathcal{K}_{\Delta t} g(\mathbf{x}_k) = g(\mathbf{F}_{\Delta t}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1})$$

- Thus, the Koopman operator advances the observation of a state

$$g(\mathbf{x}_{k+1}) = \mathcal{K}_{\Delta t} g(\mathbf{x}_k)$$

- Any conserved quantity is a Koopman eigenfunction corresponding to the eigenvalue $\lambda = 0$
- The constant function $\varphi = 1$ is the trivial eigenfunction
- Product of two eigenfunctions is still an eigenfunction:

$$\begin{aligned}\mathcal{K}(\varphi_1\varphi_2) &= \frac{d}{dt}(\varphi_1\varphi_2) \\ &= \dot{\varphi}_1\varphi_2 + \varphi_1\dot{\varphi}_2 \\ &= \lambda_1\varphi_1\varphi_2 + \lambda_2\varphi_1\varphi_2 \\ &= (\lambda_1 + \lambda_2)\varphi_1\varphi_2.\end{aligned}$$

- The continuous and discrete time eigenvalues are related: if λ is a continuous time eigenvalue, then $e^{\lambda t}$ is the corresponding discrete time eigenvalue:

$$\lim_{t \rightarrow 0} \frac{\mathcal{K}_t \varphi(\mathbf{x}) - \varphi(\mathbf{x})}{t} = \lim_{t \rightarrow 0} \frac{e^{\lambda t} \varphi(\mathbf{x}) - \varphi(\mathbf{x})}{t} = \lambda \varphi(\mathbf{x})$$

We don't have eigenfunction(s) in the beginning

Koopman mode decomposition

- Usually, we like to take multiple measurements of a system
- We denote these measurements as a vector

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix}$$

- Each individual measurement can be expanded in terms of eigenfunctions

$$g_i(\mathbf{x}) = \sum_{j=1}^{\infty} v_{ij} \varphi_j(\mathbf{x})$$

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix} = \sum_{j=1}^{\infty} \varphi_j(\mathbf{x}) \mathbf{v}_j$$

where \mathbf{v}_j is the j-th Koopman mode associated with φ_j

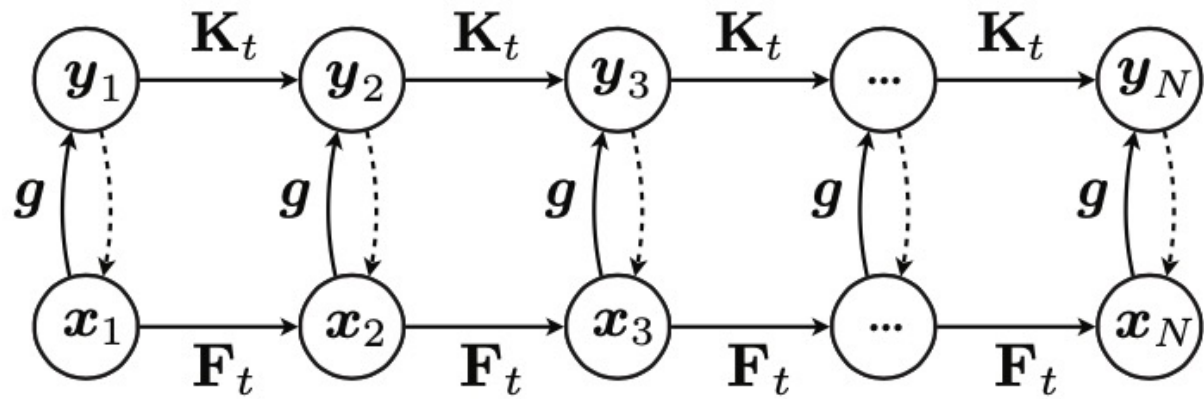
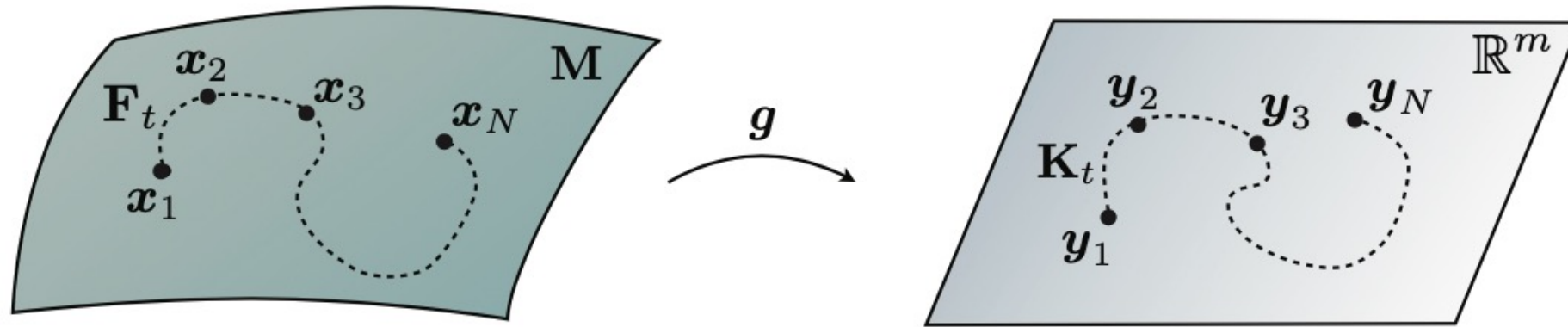
- Using the above decomposition, we can represent the dynamics of the measurement function as follows

$$\begin{aligned}\mathbf{g}(\mathbf{x}_k) &= \mathcal{K}_{\Delta t}^k \mathbf{g}(\mathbf{x}_0) = \mathcal{K}_{\Delta t}^k \sum_{j=0}^{\infty} \varphi_j(\mathbf{x}_0) \mathbf{v}_j \\ &= \sum_{i=0}^{\infty} \mathcal{K}_{\Delta t}^k \varphi_j(\mathbf{x}_0) \mathbf{v}_j \\ &= \sum_{j=0}^{\infty} \lambda_j^k \varphi_j(\mathbf{x}_0) \mathbf{v}_j\end{aligned}$$

- The triple $\{(\lambda_j, \varphi_j, \mathbf{v}_j)\}_{j=0}^{\infty}$ is called the **Koopman mode decomposition**

Koopman mode
eigenvalues
eigenvectors
eigenfunctions

- Schematic for Koopman operator



$$F_t: x_k \mapsto x_{k+1}$$

$$g: x_k \mapsto y_k$$

$$K_t: y_k \mapsto y_{k+1}$$

(invariant: after mapping, you are still within the subspace)

Invariant eigenspace

- A **Koopman invariant subspace** is the span of functions $\{g_1, g_2, \dots, g_p\}$ if all functions g in this space

$$g = \alpha_1 g_1 + \alpha_2 g_2 + \dots + \alpha_p g_p$$

remain in the space after applied the Koopman operator

$$\mathcal{K}g = \beta_1 g_1 + \beta_2 g_2 + \dots + \beta_p g_p$$

- Find a finite dimensional matrix representation of the Koopman operator restricted to the invariant subspace
- This gives finite dimensional systems

$$g(\mathbf{x}_{k+1}) = \mathcal{K}_{\Delta t} g(\mathbf{x}_k) \qquad \frac{d}{dt}g = \mathcal{K}g.$$

A simple example

- Consider the following nonlinear dynamical system

$$\dot{x}_1 = \mu x_1$$

$$\dot{x}_2 = \lambda(x_2 - x_1^2)$$

- We introduce the nonlinear measurement $g = x_1^2$

$$\frac{d}{dt} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \quad \text{for} \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix}$$

Examples of Koopman eigenfunctions

- Consider the linear dynamics

$$\frac{d}{dt}x = x$$

- Using Taylor's expansion

$$\varphi(x) = c_0 + c_1x + c_2x^2 + c_3x^3 + \dots$$

$$\nabla\varphi = c_1 + 2c_2x + 3c_3x^2 + 4c_4x^3 + \dots$$

$$\nabla\varphi \cdot f = c_1x + 2c_2x^2 + 3c_3x^3 + 4c_4x^4 + \dots$$

- We use the equation $\nabla\varphi(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = \lambda\varphi(\mathbf{x})$
- We observe that $c_0 = 0$

- For any positive integer $\lambda = k$, $\varphi(x) = cx^k$ is an eigenfunction

???

- Consider the nonlinear dynamical system

$$\frac{d}{dt} = x^2$$

- Assume the Laurent series

$$\begin{aligned}\varphi(x) = & \cdots + c_{-3}x^{-3} + c_{-2}x^{-2} + c_{-1}x^{-1} + c_0 \\ & + c_1x + c_2x^2 + c_3x^3 + \cdots .\end{aligned}$$

$$\begin{aligned}\nabla\varphi = & \cdots - 3c_{-3}x^{-4} - 2c_{-2}x^{-3} - c_{-1}x^{-2} + c_1 + 2c_2x \\ & + 3c_3x^2 + 4c_4x^3 + \cdots\end{aligned}$$

$$\begin{aligned}\nabla\varphi \cdot f = & \cdots - 3c_{-3}x^{-2} - 2c_{-2}x^{-1} - c_{-1} + c_1x^2 + 2c_2x^3 \\ & + 3c_3x^4 + 4c_4x^5 + \cdots .\end{aligned}$$

- We observe $c_k = 0$ for $k \geq 1$, and $\lambda c_{k+1} = kc_k$ for $k \leq -1$

- Thus, for any $\lambda \in \mathbb{C}$, we have

$$\varphi(x) = c_0 \left(1 - \lambda x^{-1} + \frac{\lambda^2}{2} x^{-2} - \frac{\lambda^3}{3} x^{-3} + \cdots \right) = c_0 e^{-\lambda/x}$$

Extended DMD: data-driven approach

- Goal: identify Koopman eigenfunctions from data
- We construct an augmented state

$$\mathbf{y} = \mathbf{\Theta}^T(\mathbf{x}) = \begin{bmatrix} \theta_1(\mathbf{x}) \\ \theta_2(\mathbf{x}) \\ \vdots \\ \theta_p(\mathbf{x}) \end{bmatrix}$$

which contains the original state and nonlinear measurements, $p \gg n$

- Define the data matrices

$$\mathbf{Y} = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_m \\ | & | & \cdots & | \end{bmatrix}, \quad \mathbf{Y}' = \begin{bmatrix} | & | & \cdots & | \\ \mathbf{y}_2 & \mathbf{y}_3 & \cdots & \mathbf{y}_{m+1} \\ | & | & \cdots & | \end{bmatrix}$$

- The best fit matrix is obtained by

$$\mathbf{A}_{\mathbf{Y}} = \underset{\mathbf{A}_{\mathbf{Y}}}{\operatorname{argmin}} \|\mathbf{Y}' - \mathbf{A}_{\mathbf{Y}}\mathbf{Y}\| = \mathbf{Y}'\mathbf{Y}^\dagger$$

- Equivalently

$$\mathbf{A}_{\mathbf{Y}} = \underset{\mathbf{A}_{\mathbf{Y}}}{\operatorname{argmin}} \|\boldsymbol{\Theta}^T(\mathbf{X}') - \mathbf{A}_{\mathbf{Y}}\boldsymbol{\Theta}^T(\mathbf{X})\| = \boldsymbol{\Theta}^T(\mathbf{X}') \left(\boldsymbol{\Theta}^T(\mathbf{X}) \right)^\dagger$$

Approximating Koopman eigenfunctions

- For discrete time dynamics, Koopman eigenfunction satisfies

$$\begin{bmatrix} \lambda \varphi(\mathbf{x}_1) \\ \lambda \varphi(\mathbf{x}_2) \\ \vdots \\ \lambda \varphi(\mathbf{x}_m) \end{bmatrix} = \begin{bmatrix} \varphi(\mathbf{x}_2) \\ \varphi(\mathbf{x}_3) \\ \vdots \\ \varphi(\mathbf{x}_{m+1}) \end{bmatrix}$$

- Expand the eigenfunction in terms of some candidate functions

$$\Theta(\mathbf{x}) = [\theta_1(\mathbf{x}) \quad \theta_2(\mathbf{x}) \quad \cdots \quad \theta_p(\mathbf{x})] \quad \text{set of basis}$$

- So, we have

$$\varphi(\mathbf{x}) \approx \sum_{k=1}^p \theta_k(\mathbf{x}) \xi_k = \Theta(\mathbf{x}) \boldsymbol{\xi}$$

- We obtain the following using the above

$$(\lambda \Theta(\mathbf{X}) - \Theta(\mathbf{X}')) \xi = \mathbf{0}.$$

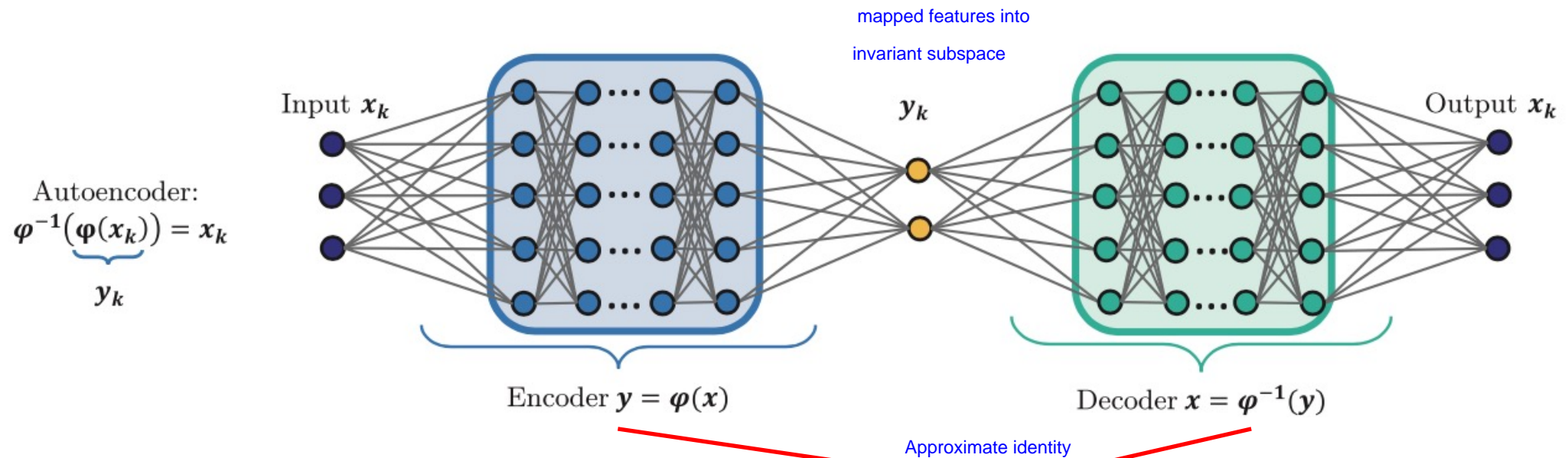
- If we seek the least squares fit

$$\lambda \xi = \Theta(\mathbf{X})^\dagger \Theta(\mathbf{X}') \xi$$

- So, we need to find eigenvectors of the above matrix

Using neural networks

- The eigenfunctions of the Koopman operator are complicated
- Deep learning provides a convincing approach
- The auto encoder structure is used naturally, that is, a few latent variables $\mathbf{y} = \boldsymbol{\varphi}(\mathbf{x})$ are used to parameterize the dynamics



- An additional constraint is enforced so that the dynamic is linear on these latent variables
- This constraint can be enforced using the loss function $\|\varphi(\mathbf{x}_{k+1}) - \mathbf{K}\varphi(\mathbf{x}_k)\|$ where K is a matrix

