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# Data-Driven Discovery of Koopman Embeddings for Spatio-Temporal Systems

**SIAM DS 2019**

*Advanced Data-Driven Techniques and Numerical Methods in  
Koopman Operator Theory*



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**arXiv (2019)**

# Bernard Koopman 1931

**Definition:** Koopman Operator (Koopman 1931): *For a dynamical system*

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

*where  $\mathbf{x} \in \mathbb{R}^n$  is in a state space  $\mathbf{x} \in \mathcal{M}$ . The Koopman operator  $\mathcal{K}$  acts on a set of scalar observable variables  $g_j$  which comprise the vector  $\mathbf{g}: \mathcal{M} \rightarrow \mathbb{C}$  so that*

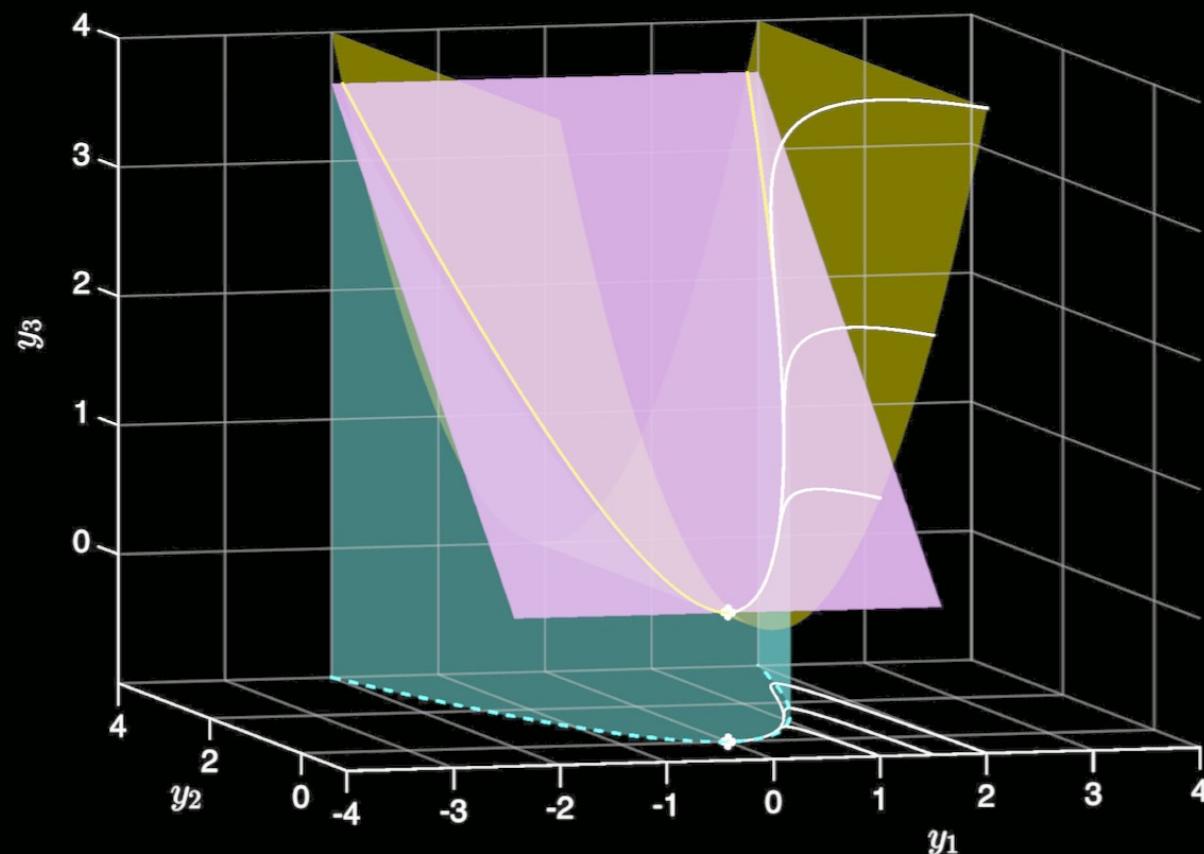
$$\mathcal{K}\mathbf{g}(\mathbf{x}) = \mathbf{g}(\mathbf{N}(\mathbf{x})).$$

**Mezic (2004), Schmid (2010), Rowley et al (2009)**  
**Coifman, Kevrekidis, co-workers - Diffusion Maps**  
**Williams et al - EDMD**

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# Koopman Invariant Subspaces

$$\left. \begin{array}{l} \dot{x}_1 = \mu x_1 \\ \dot{x}_2 = \lambda(x_2 - x_1^2) \end{array} \right\} \implies \frac{d}{dt} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \quad \text{for} \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 \end{bmatrix}$$



Brunton, Proctor & Kutz, PLOS ONE (2018)

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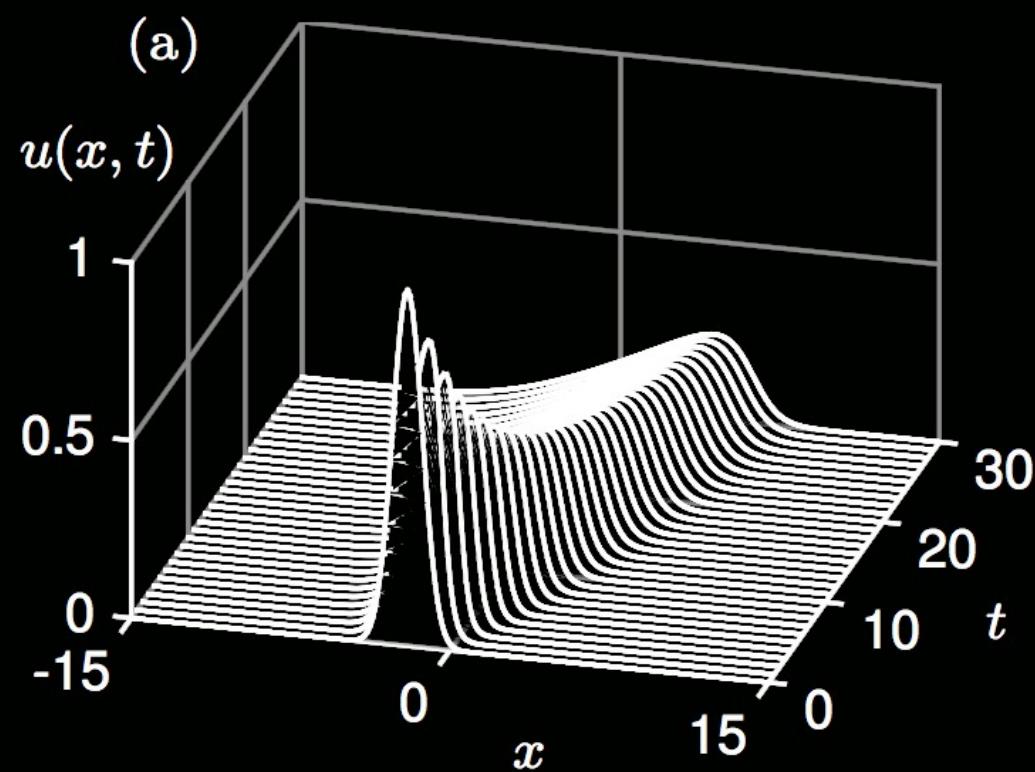
# Burgers' Equation

$$u_t + uu_x - \epsilon u_{xx} = 0 \quad \epsilon > 0, \quad x \in [-\infty, \infty]$$

Cole-Hopf

$$u = -2\epsilon v_x/v$$

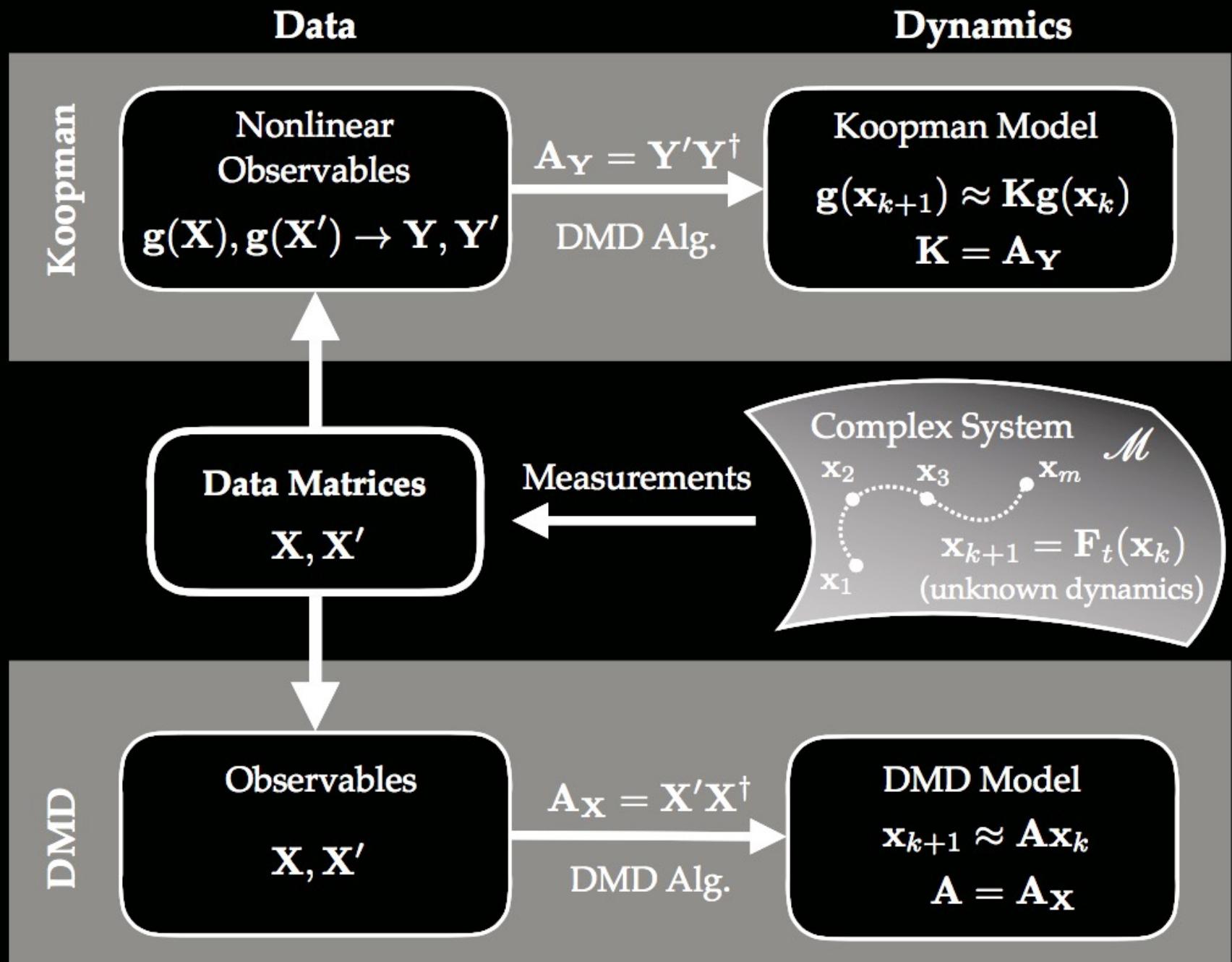
$$v_t = \epsilon v_{xx}$$



Kutz, Proctor & Brunton, Complexity (2018)

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# Koopman vs DMD: All about Observables!

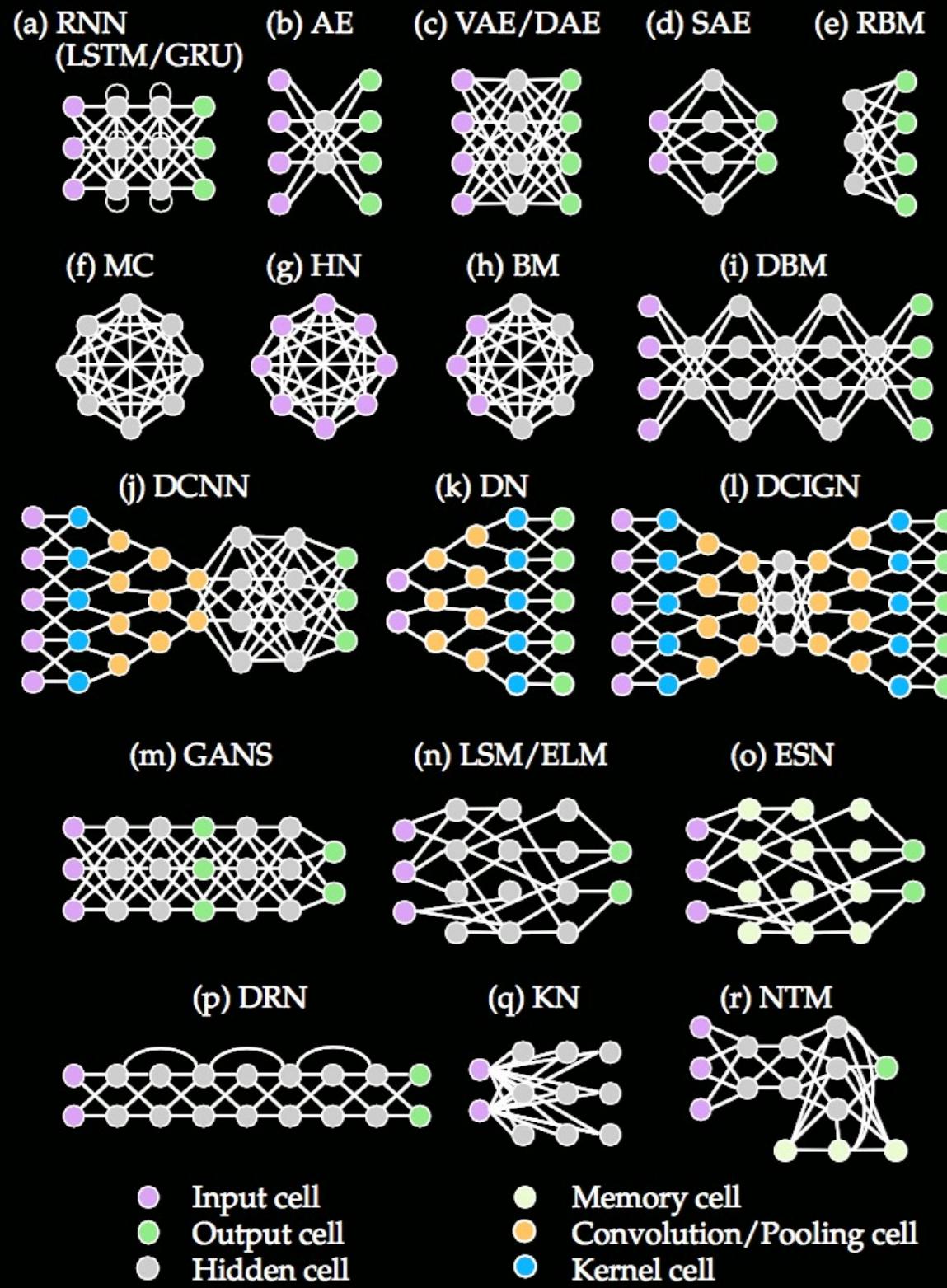


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# Neural Nets

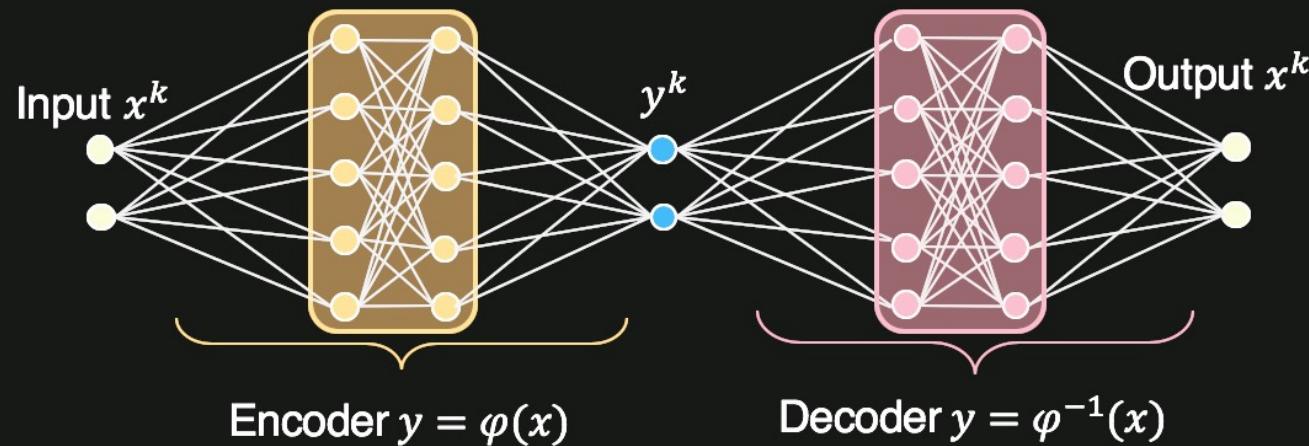
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# NN Zoo

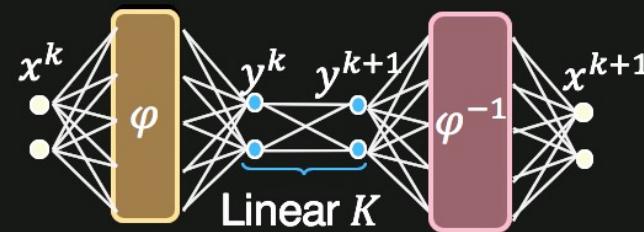


# NNs for Koopman Embedding

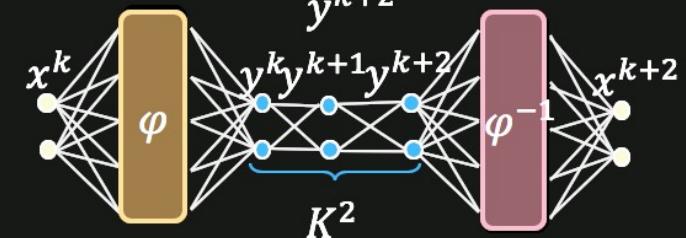
$$\text{Autoencoder: } \varphi^{-1} \left( \underbrace{\varphi(x^k)}_{y^k} \right) = x^k$$



$$\text{Prediction: } \varphi^{-1} \left( \underbrace{K\varphi(x^k)}_{y^{k+1}} \right) = x^{k+1}$$



$$\text{Prediction: } \varphi^{-1} \left( \underbrace{K^2\varphi(x^k)}_{y^{k+2}} \right) = x^{k+2}$$



Bethany Lusch

Lusch et al. Nat. Comm (2018)

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Failure!  
*(obviously)*

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# Duffing Oscillator

Poincaré-Lindstedt Expansion: let  $\tau = \omega t$  so that

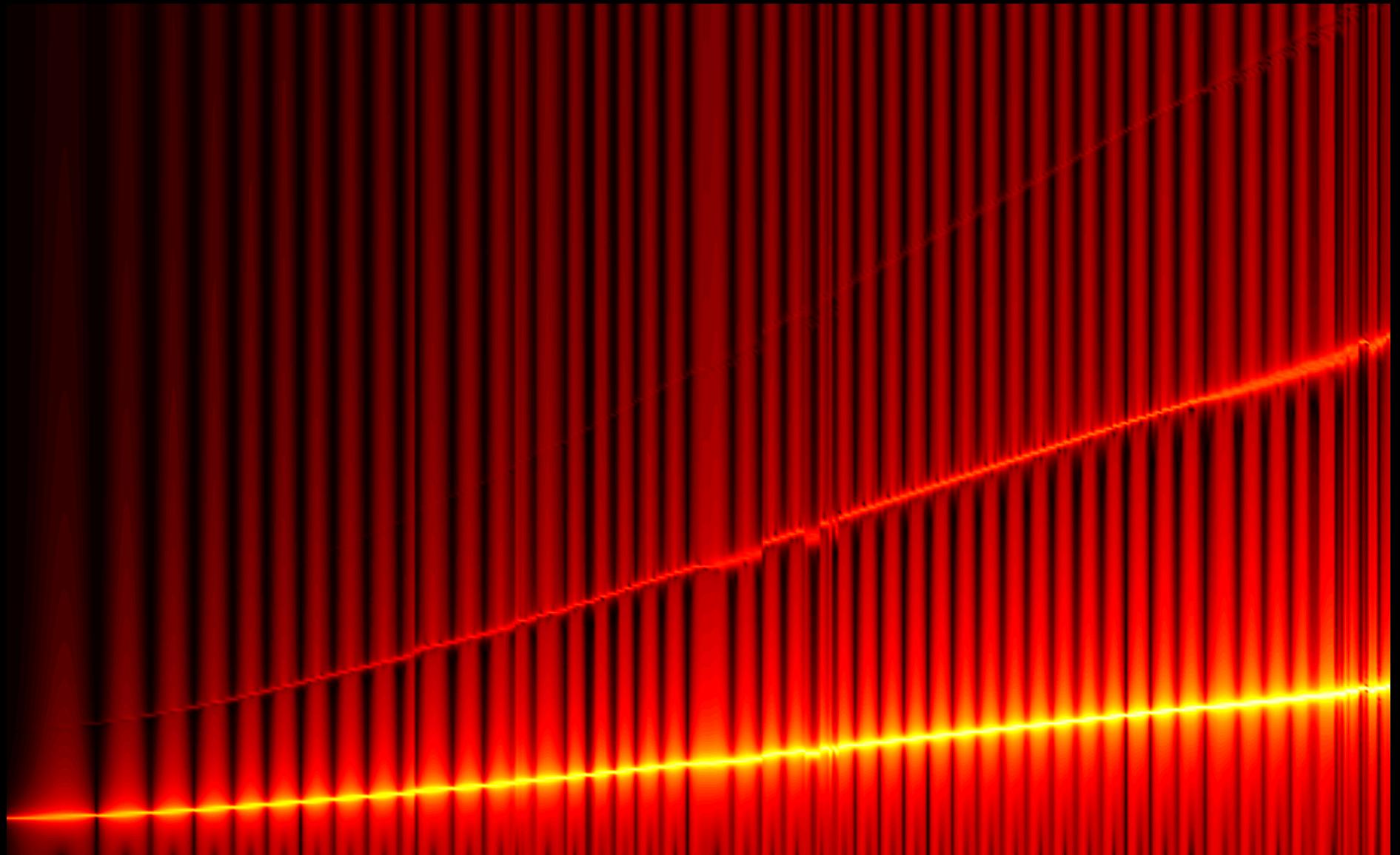
$$y_{\tau\tau} + y + \epsilon y^3 = 0 \Rightarrow \omega^2 y_{\tau\tau} + y + \epsilon y^3 = 0$$

**Nonlinearity: Shifts Frequencies + Generates Harmonics**

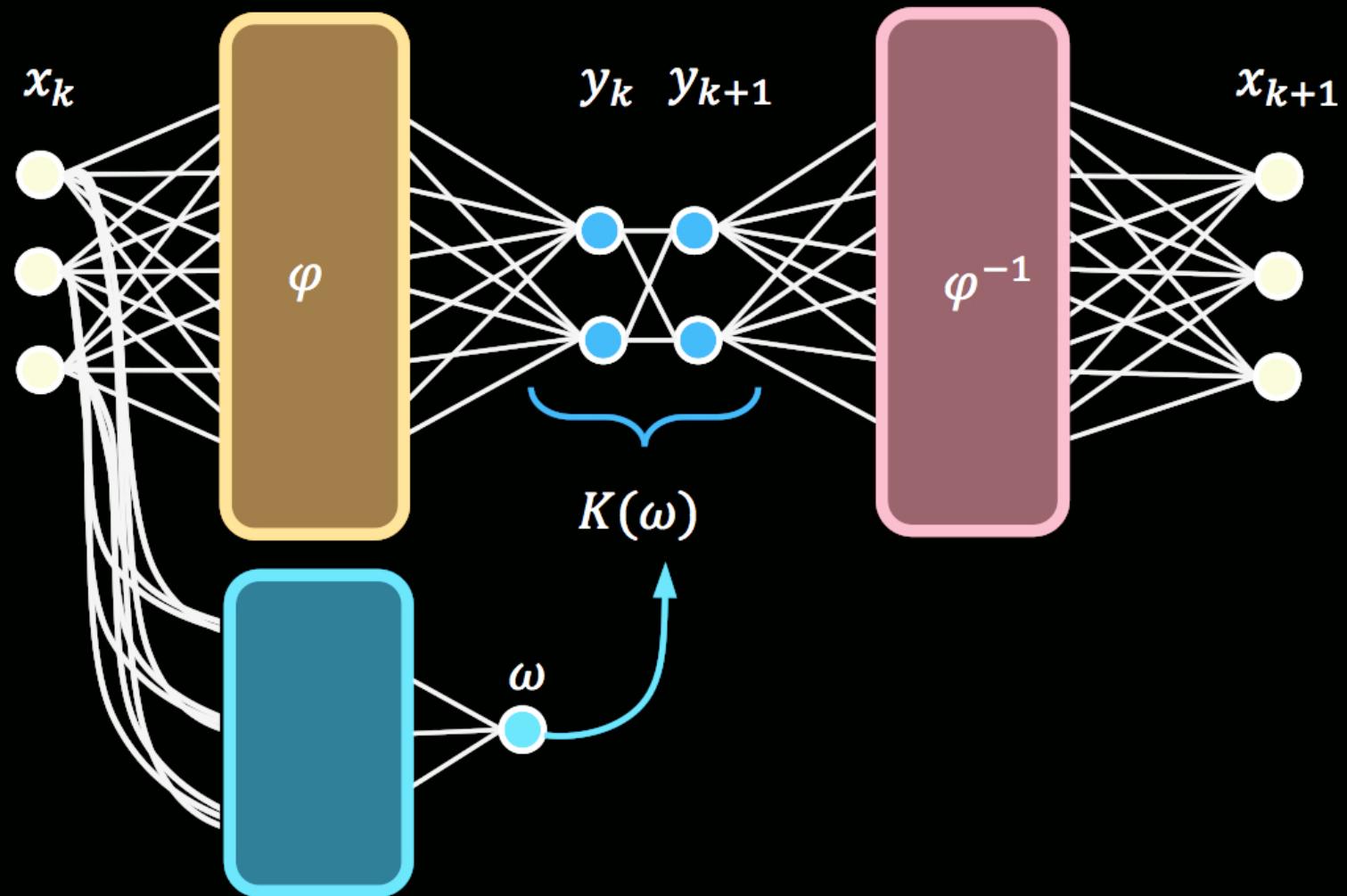
$$y = A \sin[(1+3A^2/8)t] + \epsilon \left\{ \frac{3A^3}{32} \sin\left[\left(1+\epsilon \frac{3A^2}{8}\right)t\right] - \frac{A^3}{32} \sin\left[3\left(1+\epsilon \frac{3A^2}{8}\right)t\right] \right\}$$

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# Spectrogram



# *Handling the Continuous Spectra*

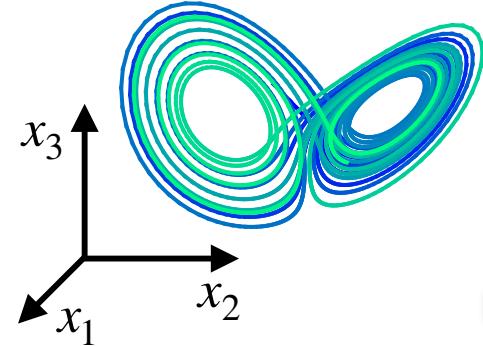


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Relax Koopman

# Sparse Identification of Nonlinear Dynamics (SINDy)

True System



$$\dot{x}_1 = \sigma(x_2 - x_1)$$

$$\dot{x}_2 = x_1(\rho - x_3) - x_2$$

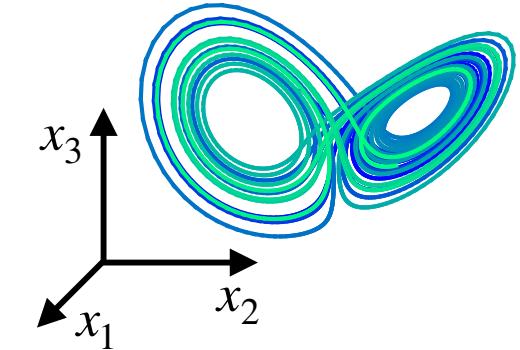
$$\dot{x}_3 = x_1x_2 - \beta x_3$$

SINDy fitting

$$\begin{bmatrix} \dot{x}_1 & \dot{x}_2 & \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_2 & x_3 & x_1^2 & x_1x_2 & x_3^3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \xi_1 & \xi_2 & \xi_3 \end{bmatrix}$$

The diagram illustrates the SINDy fitting process. On the left, the true system's dynamics are shown as a set of differential equations. An arrow points to the middle, where the data matrix  $\dot{\mathbf{X}}$  is shown as a column vector of derivatives, and the feature matrix  $\Theta(\mathbf{X})$  is shown as a matrix of powers of the state variables  $x_1, x_2, x_3$ . A second arrow points to the right, where the identified system's dynamics are shown as a sparse matrix  $\Xi$  connecting the features to the identified parameters  $\xi_1, \xi_2, \xi_3$ .

Identified System

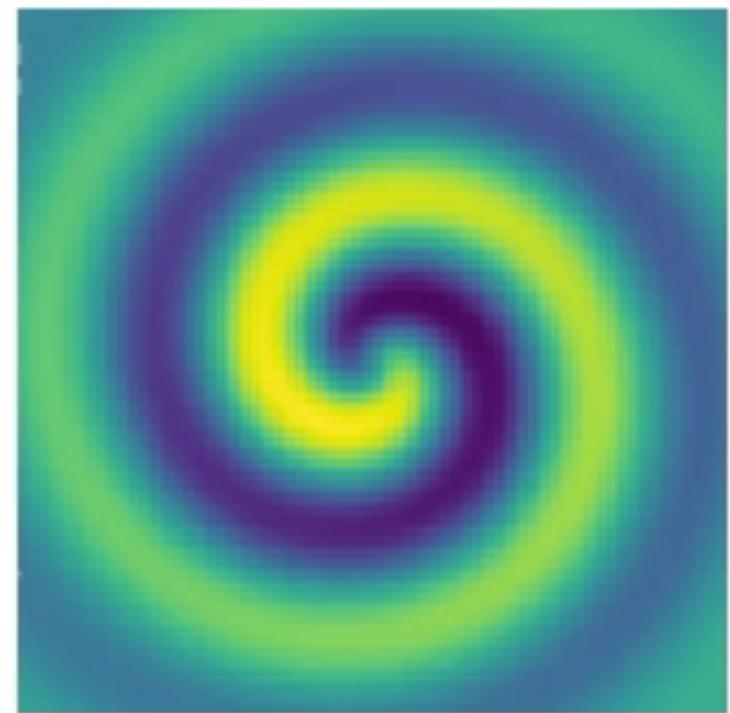
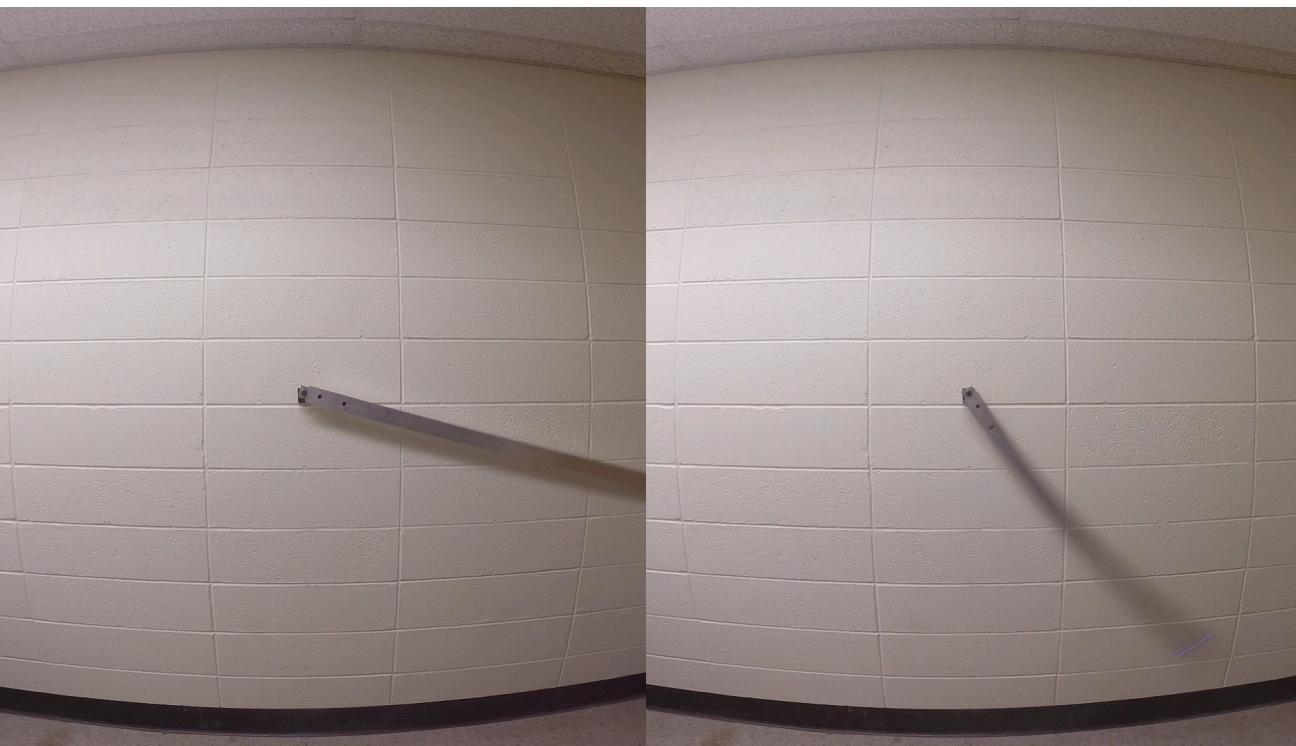


$$\dot{x}_1 = \Theta(\mathbf{x}^T)\xi_1$$

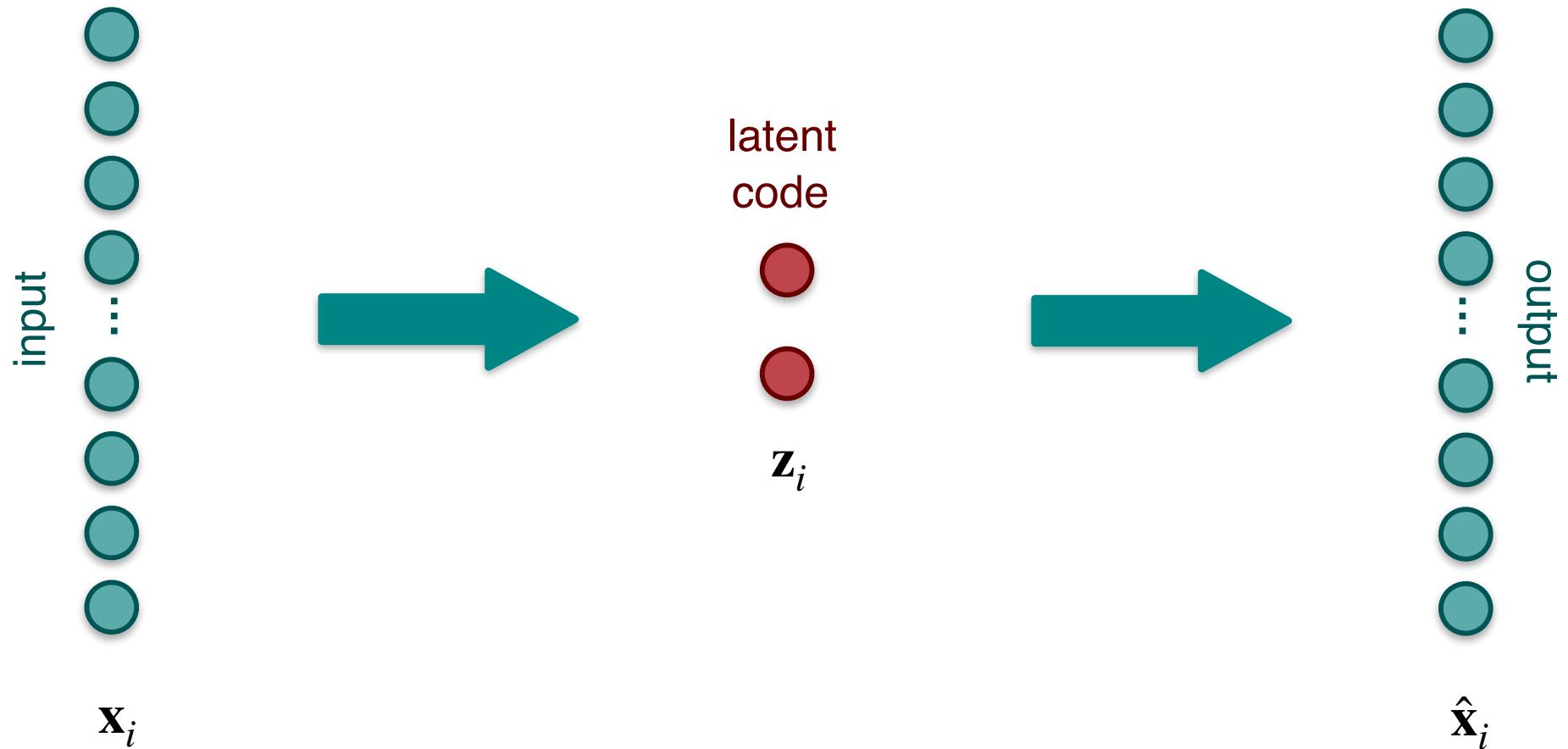
$$\dot{x}_2 = \Theta(\mathbf{x}^T)\xi_2$$

$$\dot{x}_3 = \Theta(\mathbf{x}^T)\xi_3$$

# What if we don't know the right coordinates?

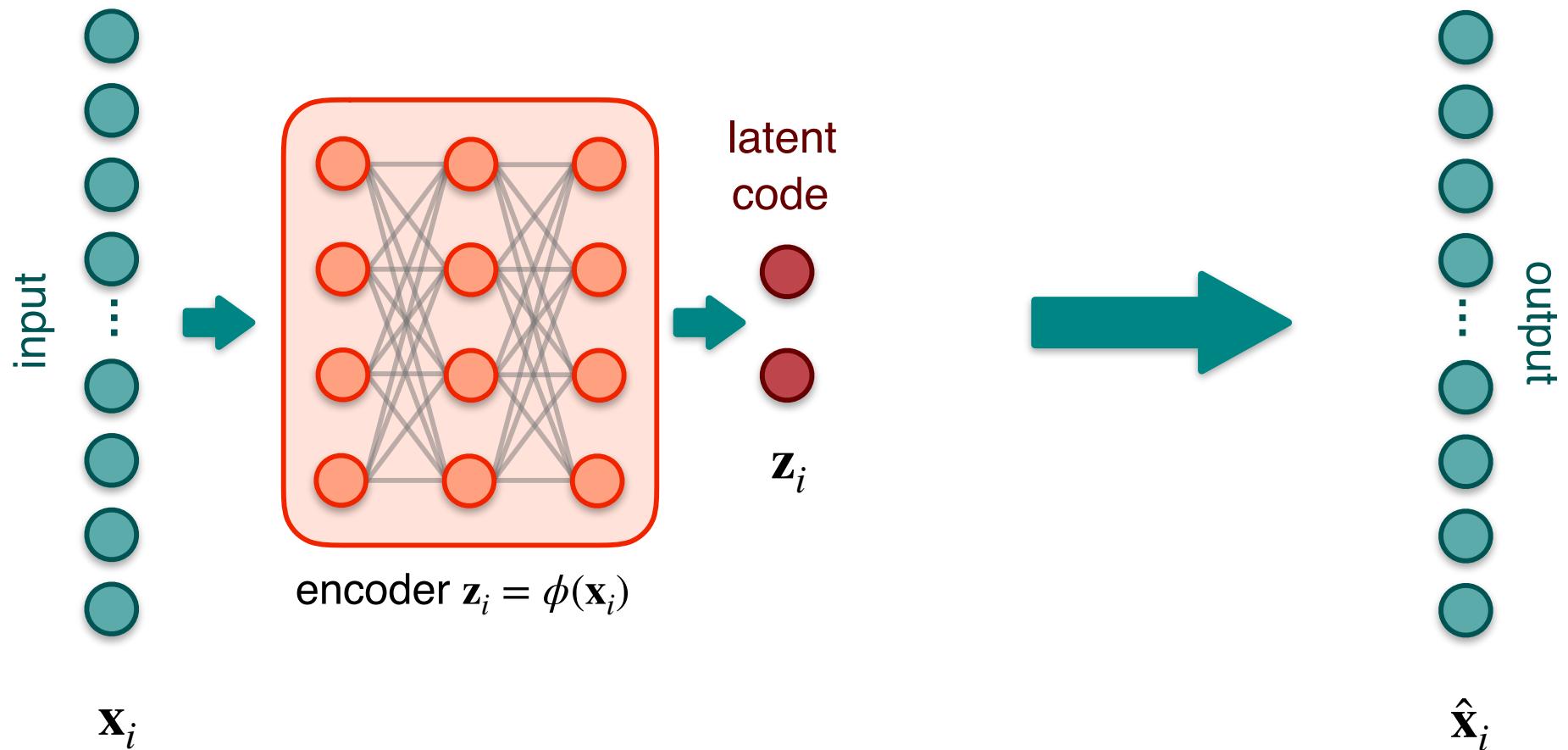


# Autoencoder



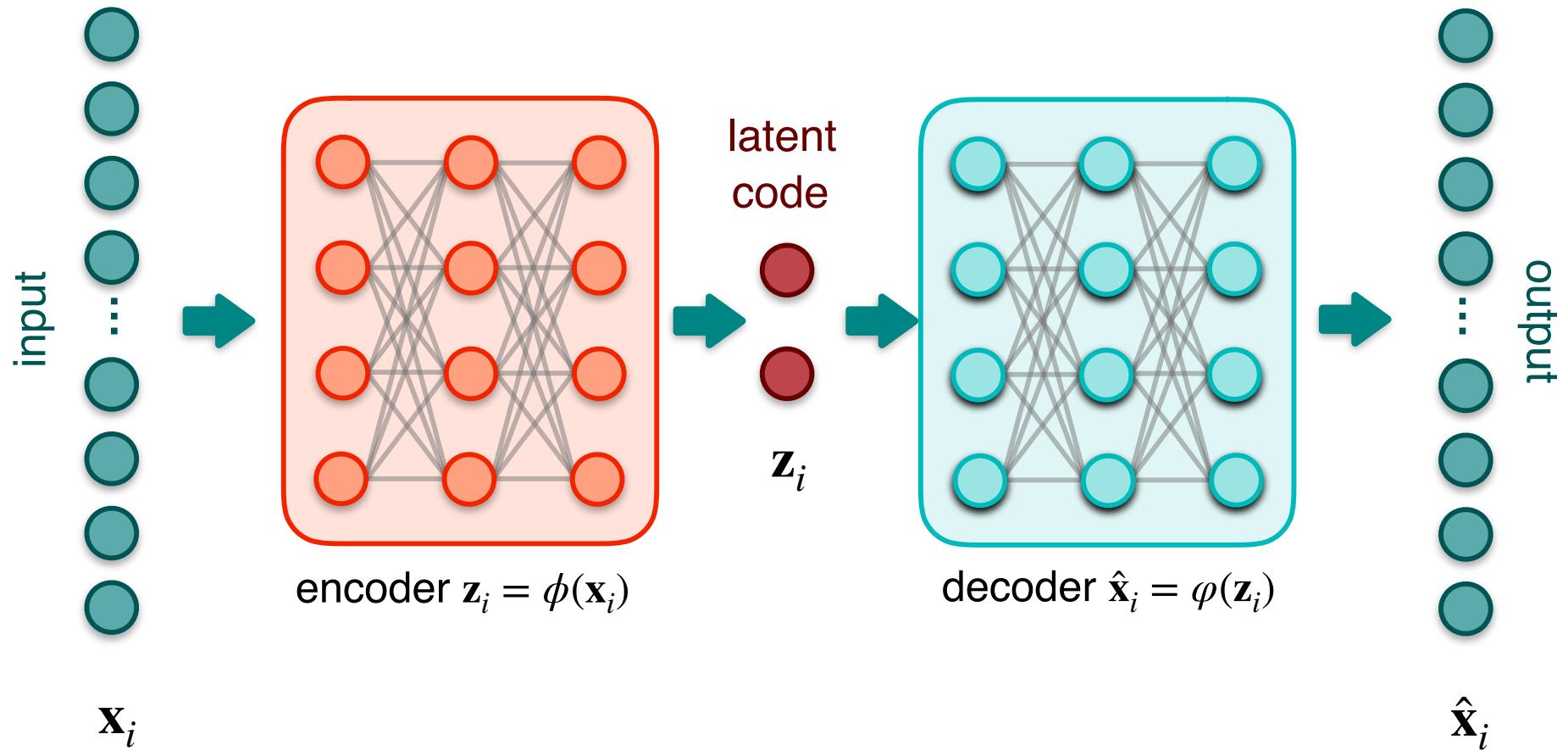
**loss function:** 
$$\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$$

# Autoencoder



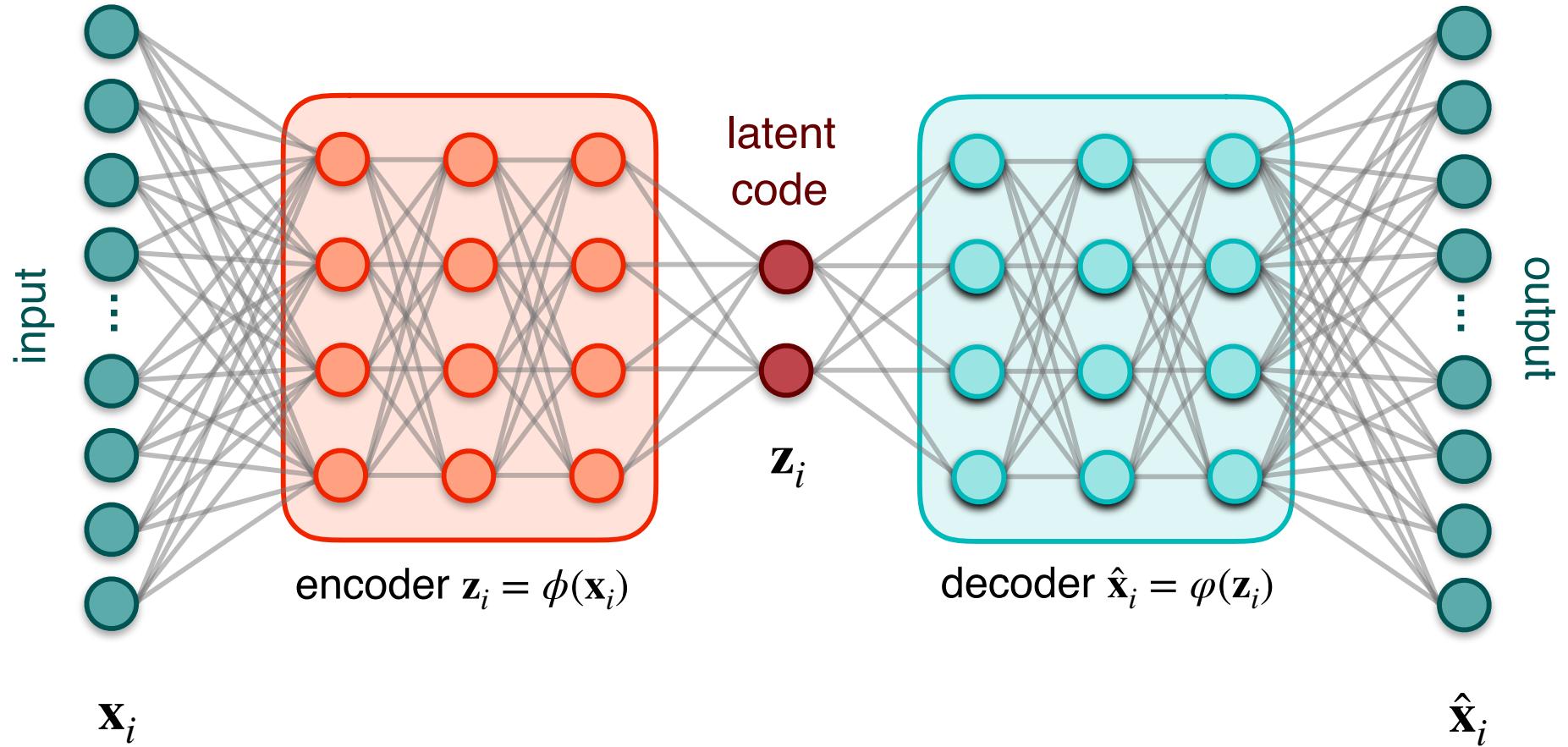
**loss function:** 
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# Autoencoder



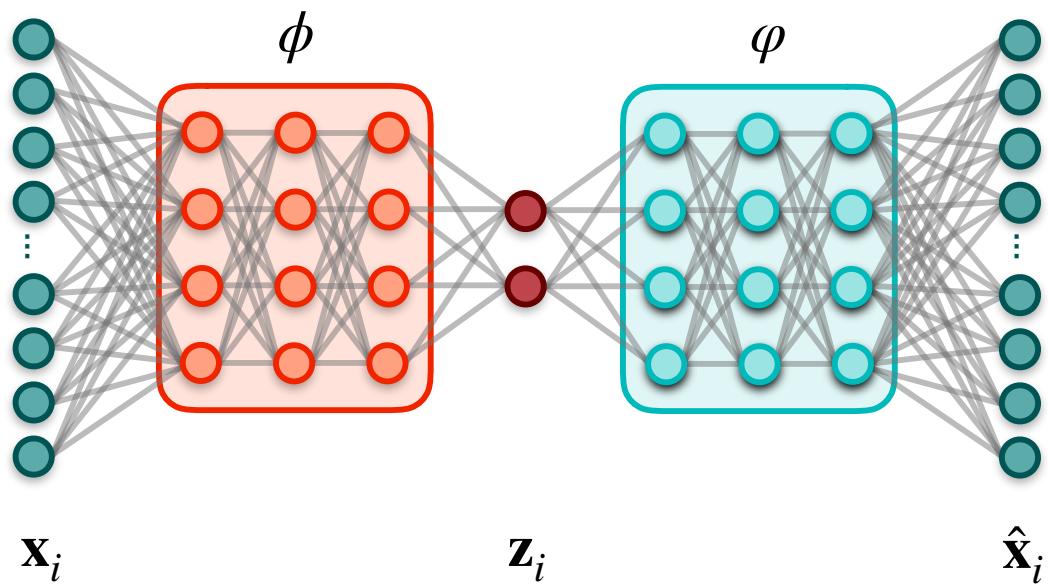
**loss function:** 
$$\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$$

# Autoencoder



**loss function:**  $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

# Autoencoder + SINDy

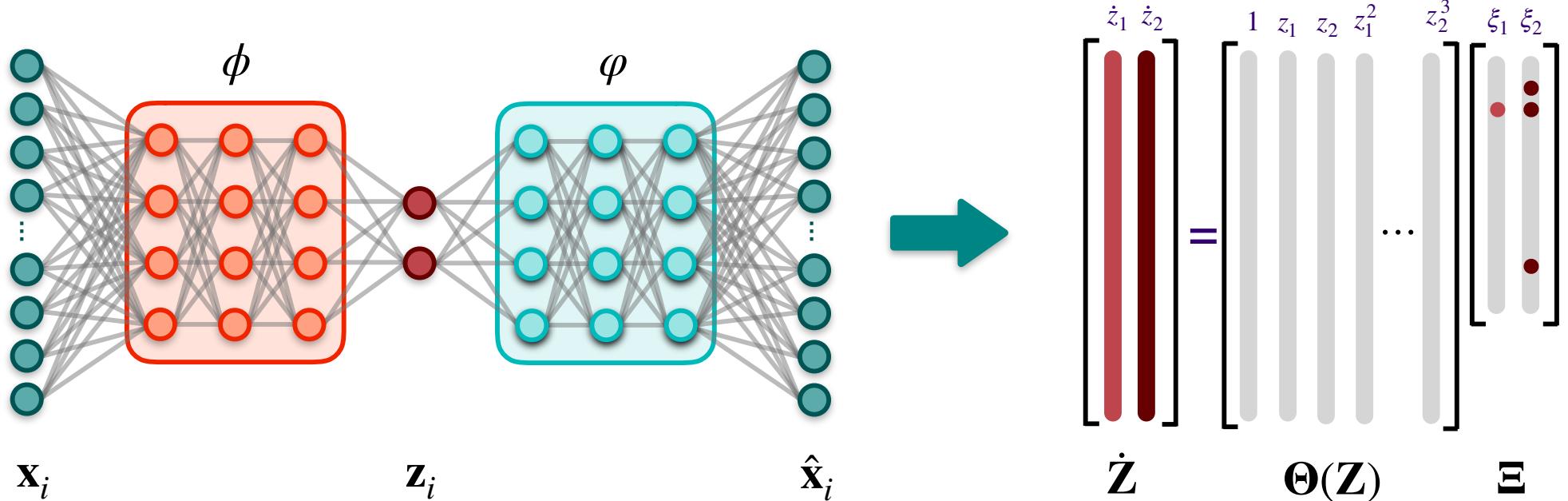


$$\begin{bmatrix} \dot{z}_1 & \dot{z}_2 \end{bmatrix} = \begin{bmatrix} 1 & z_1 & z_2 & z_1^2 \end{bmatrix} \dots = \begin{bmatrix} z_2^3 & \xi_1 & \xi_2 \end{bmatrix} [\Theta(\mathbf{Z}) \quad \mathbf{E}]$$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2$

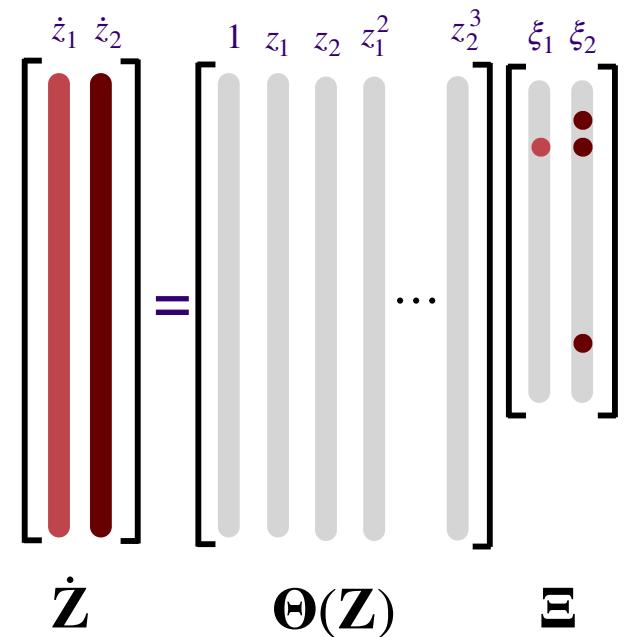
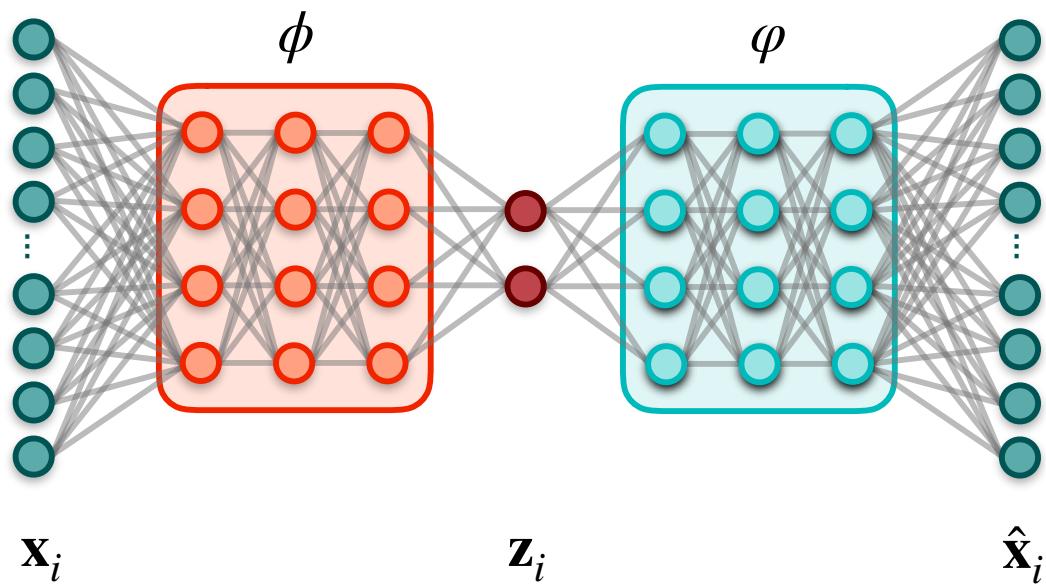
# Autoencoder + SINDy



**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2$

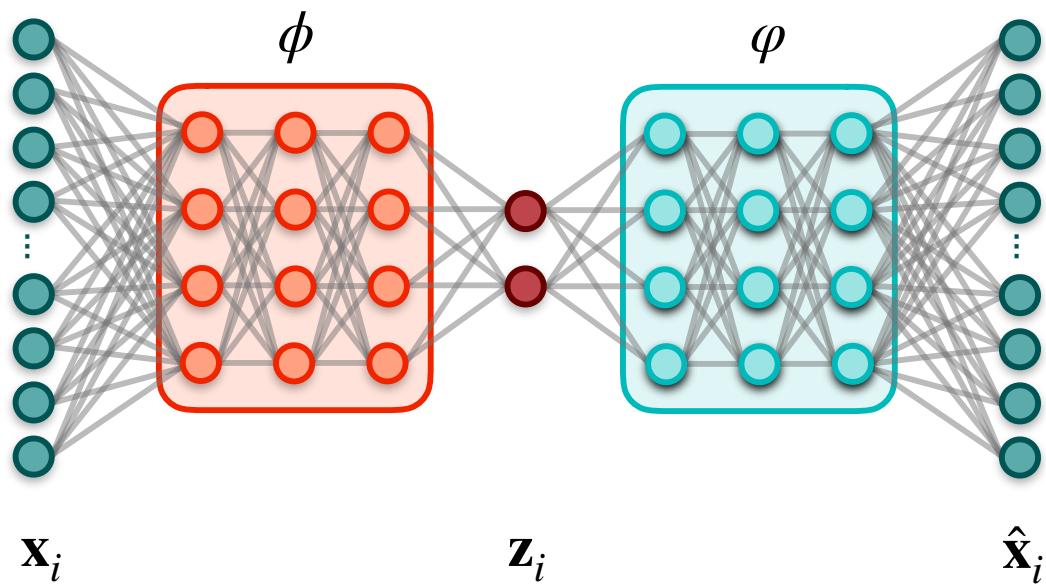
# Autoencoder + SINDy



**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \mathbf{E}\|_2^2$

# Autoencoder + SINDy



$$\begin{bmatrix} \dot{z}_1 & \dot{z}_2 \end{bmatrix} = \begin{bmatrix} 1 & z_1 & z_2 & z_1^2 & z_2^3 & \xi_1 & \xi_2 \end{bmatrix} \begin{bmatrix} \dots \\ \vdots \end{bmatrix}$$

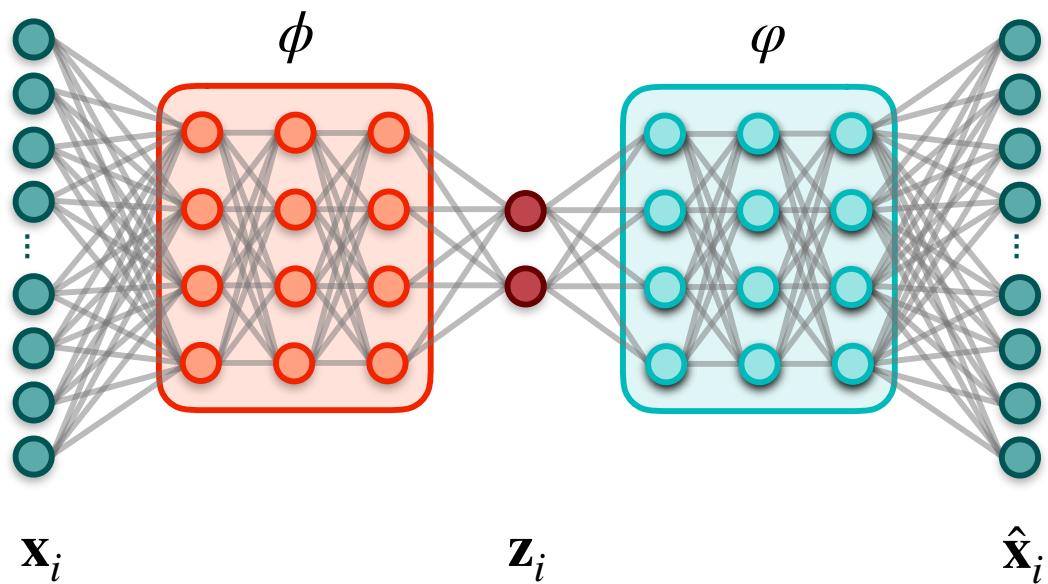
The diagram shows the state-space representation of the system. The leftmost column contains two red vertical bars labeled  $\dot{z}_1$  and  $\dot{z}_2$ . To its right is an equals sign. Further right is a large bracket containing several gray vertical bars. These bars are labeled at the top with the values 1,  $z_1$ ,  $z_2$ ,  $z_1^2$ ,  $z_2^3$ ,  $\xi_1$ , and  $\xi_2$ . Below this large bracket is the label  $\Theta(\mathbf{Z})$ . To the right of the large bracket is another large bracket containing two small red vertical bars labeled  $\xi_1$  and  $\xi_2$ . Below this second large bracket is the label  $\Xi$ .

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2$

$$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}} \phi(\mathbf{x}_i) \dot{\mathbf{x}}_i$$

# Autoencoder + SINDy



$$\begin{bmatrix} \dot{z}_1 & \dot{z}_2 \end{bmatrix} = \begin{bmatrix} 1 & z_1 & z_2 & z_1^2 & z_2^3 & \xi_1 & \xi_2 \end{bmatrix} \begin{bmatrix} \dots \\ \vdots \end{bmatrix}$$

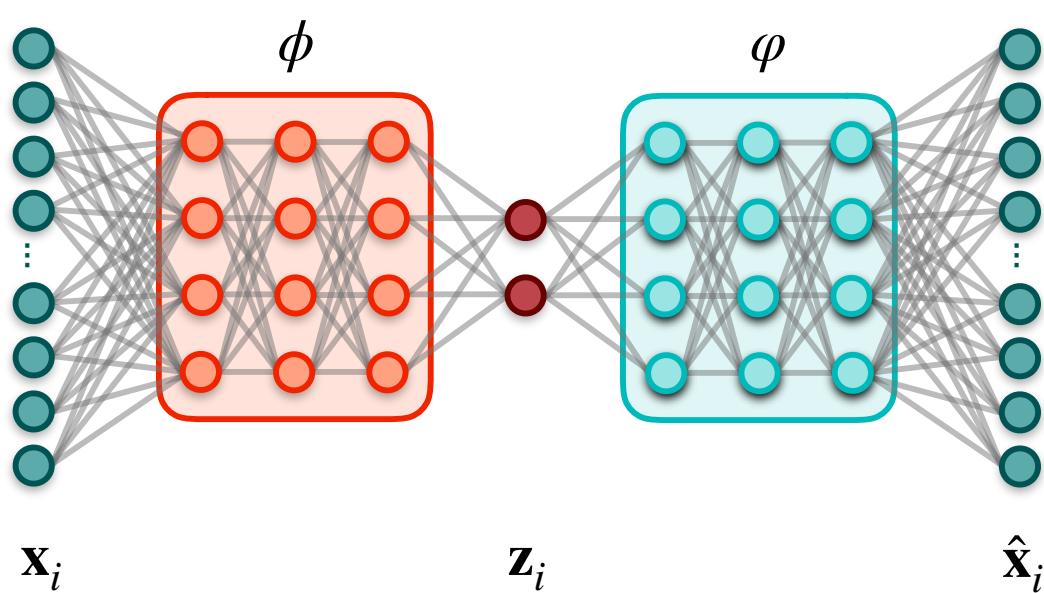
$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}} \phi(\mathbf{x}_i) \dot{\mathbf{x}}_i$

$\Theta(\mathbf{z}_i^T) = \Theta(\phi(\mathbf{x}_i)^T)$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

**loss:**  $\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2$

# Autoencoder + SINDy



$$\begin{bmatrix} \dot{z}_1 & \dot{z}_2 \end{bmatrix} = \begin{bmatrix} 1 & z_1 & z_2 & z_1^2 \\ \dots & \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} z_2^3 & \xi_1 & \xi_2 \end{bmatrix}$$

$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}} \phi(\mathbf{x}_i) \dot{\mathbf{x}}_i$

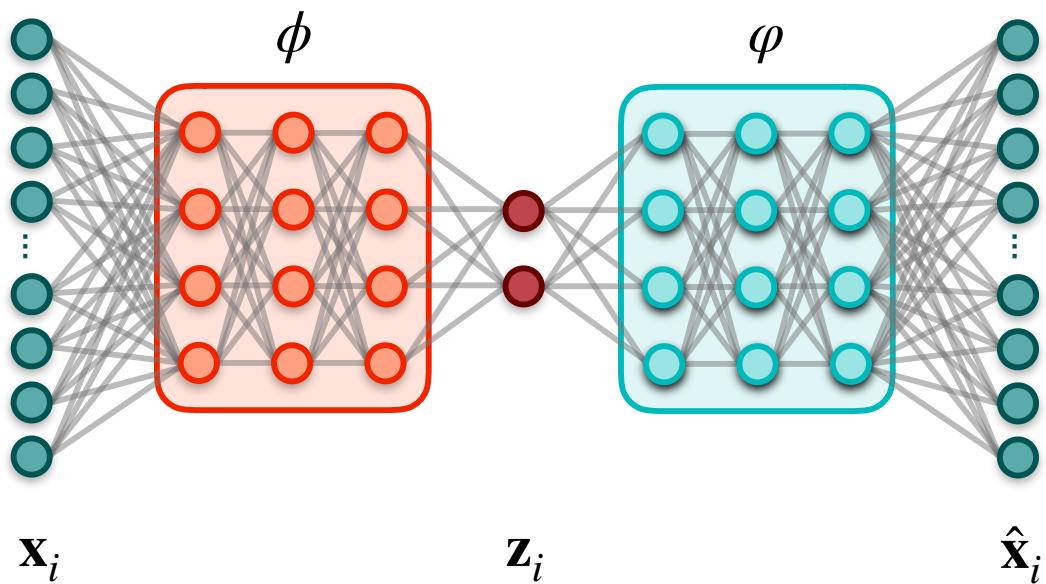
$\Theta(\mathbf{z}_i^T) = \Theta(\phi(\mathbf{x}_i)^T) \Xi$

**loss:**  $\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \varphi(\phi(\mathbf{x}_i))\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\nabla_{\mathbf{x}} \phi(\mathbf{x}_i) \dot{\mathbf{x}}_i - \Theta(\phi(\mathbf{x}_i)^T) \Xi\|_2^2$

**autoencoder  
component**

**SINDy  
component**

# Autoencoder + SINDy



$$\begin{bmatrix} \dot{z}_1 & \dot{z}_2 \end{bmatrix} = \begin{bmatrix} 1 & z_1 & z_2 & z_1^2 \\ \dots & \dots & \dots & \dots \end{bmatrix} \begin{bmatrix} z_2^3 & \xi_1 & \xi_2 \end{bmatrix}$$

$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}} \phi(\mathbf{x}_i) \dot{\mathbf{x}}_i$

$\Theta(\mathbf{z}_i^T) = \Theta(\phi(\mathbf{x}_i)^T)$

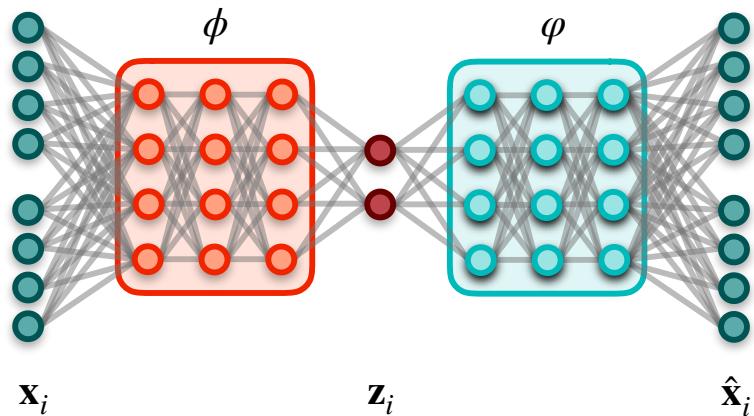
$\Xi$

**loss:**  $\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \varphi(\phi(\mathbf{x}_i))\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\nabla_{\mathbf{x}} \phi(\mathbf{x}_i) \dot{\mathbf{x}}_i - \Theta(\phi(\mathbf{x}_i)^T) \Xi\|_2^2 + \lambda_3 \|\Xi\|_1$

**autoencoder  
component**

**SINDy  
component**

# Autoencoder + SINDy



**loss:**

$$\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2 + \lambda_3 \|\Xi\|_1$$

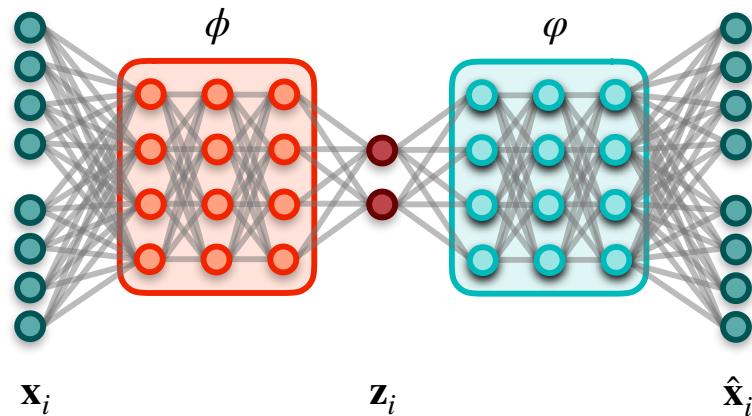
$L_1$

$L_2$

$L_3$

> **Issue:** training shrinks norm of  $\mathbf{z}$  to minimize loss function

# Autoencoder + SINDy



**loss:**

$$\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2 + \lambda_3 \|\Xi\|_1$$

$L_1$

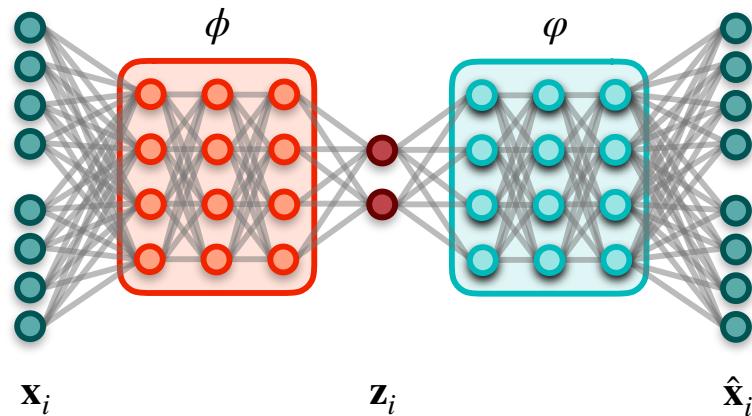
$L_2$

$L_3$

- > **Issue:** training shrinks norm of  $\mathbf{z}$  to minimize loss function
- > **Solution:** use the following to enforce SINDy loss

new  $L_2$  : 
$$\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{x}}_i - \nabla_{\mathbf{z}} \varphi(\mathbf{z}_i) \Theta(\mathbf{z}_i^T) \Xi\|_2^2 = \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{x}}_i - \nabla_{\mathbf{z}} \varphi(\phi(\mathbf{x}_i)) \Theta(\phi(\mathbf{x}_i)^T) \Xi\|_2^2$$

# Autoencoder + SINDy



**loss:**

$$\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{z}}_i - \Theta(\mathbf{z}_i^T) \Xi\|_2^2 + \lambda_3 \|\Xi\|_1$$

$L_1$

$L_2$

$L_3$

- > **Issue:** training shrinks norm of  $\mathbf{z}$  to minimize loss function
- > **Solution:** use the following to enforce SINDy loss

new  $L_2$  : 
$$\frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{x}}_i - \nabla_{\mathbf{z}} \varphi(\mathbf{z}_i) \Theta(\mathbf{z}_i^T) \Xi\|_2^2 = \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{x}}_i - \nabla_{\mathbf{z}} \varphi(\phi(\mathbf{x}_i)) \Theta(\phi(\mathbf{x}_i)^T) \Xi\|_2^2$$

> New loss function:

$$\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{x}}_i - \nabla_{\mathbf{z}} \varphi(\mathbf{z}_i) \Theta(\mathbf{z}_i^T) \Xi\|_2^2 + \lambda_3 \|\Xi\|_1$$

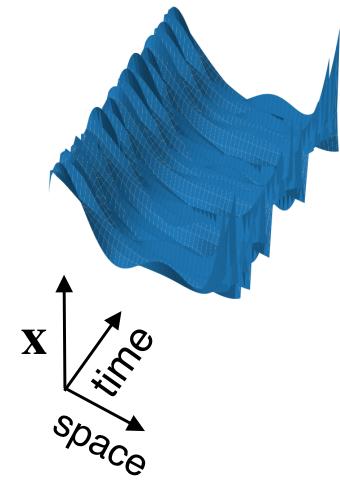
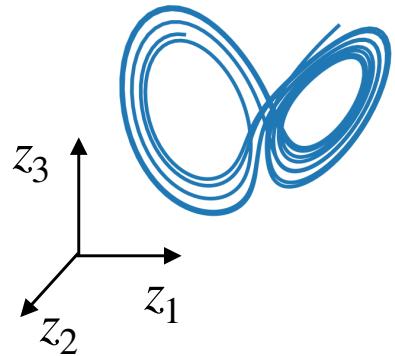
# Achieving sparsity

- > With L1 penalty alone, get model that has many very small coefficients but is not truly sparse

$$\lambda_1 \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2 + \lambda_2 \frac{1}{N} \sum_{i=1}^N \|\dot{\mathbf{x}}_i - \nabla_{\mathbf{z}} \varphi(\mathbf{z}_i) \boldsymbol{\Theta}(\mathbf{z}_i^T) \boldsymbol{\Xi}\|_2^2 + \lambda_3 \|\boldsymbol{\Xi}\|_1$$

- > Instead combine L1 penalty with sequential thresholding

# Example problem



$$\mathbf{x}(t) = \mathbf{A}\mathbf{z}(t) + \mathbf{B} \begin{pmatrix} z_1^3(t) \\ z_2^3(t) \\ z_3^3(t) \end{pmatrix}$$

$$\mathbf{x}(t) \in \mathbb{R}^{128}$$

$$\mathbf{A}, \mathbf{B} \in \mathbb{R}^{128 \times 3}$$

# Example problem

## Lorenz model

$$\dot{z}_1 = -10z_1 + 10z_2$$

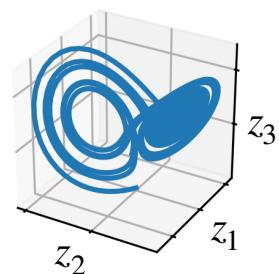
**Equations**       $\dot{z}_2 = 28z_1 - z_2 - z_1z_3$

$$\dot{z}_3 = -2.7z_3 + z_1z_2$$

**Coefficient Matrix  $\Xi$**

$$\begin{matrix} & 1 & z_1 & z_2 & z_3 & z_1^2 & \dots & z_3^3 \\ \dot{z}_1 & \boxed{\begin{matrix} 0 & 10 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix}} \\ \dot{z}_2 & \quad \quad \quad 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \dot{z}_3 & \quad \quad \quad 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix}$$

**Dynamics**



# Example problem

## Lorenz model

$$\dot{z}_1 = -10z_1 + 10z_2$$

## Equations

$$\dot{z}_2 = 28z_1 - z_2 - z_1z_3$$

$$\dot{z}_3 = -2.7z_3 + z_1z_2$$

## Discovered model

$$\dot{z}_1 = -8.5z_2z_3$$

$$\dot{z}_2 = 9.2 - 2.9z_2 + 1.1z_1z_3$$

$$\dot{z}_3 = -8.8z_1 - 10.3z_3$$

## Discovered model (transformed)

$$\dot{z}_1 = -10.2z_1 + 8.8z_2$$

$$\dot{z}_2 = 26.7z_1 - 8.5z_1z_3$$

$$\dot{z}_3 = -2.9z_3 + 1.1z_2$$

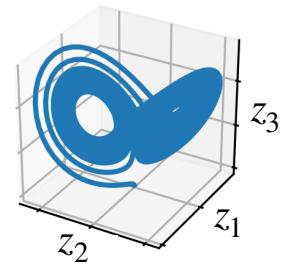
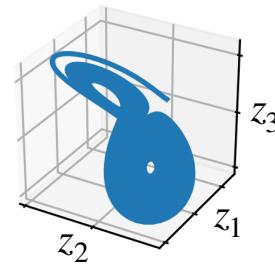
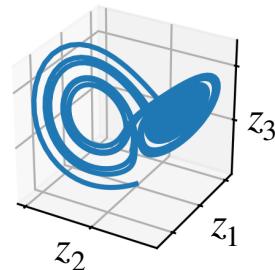
## Coefficient Matrix $\Xi$

	1	$z_1$	$z_2$	$z_3$	$z_1^2$	$z_2^2$	$z_3^2$	$\dots$
$\dot{z}_1$	1							
$\dot{z}_2$								
$\dot{z}_3$								

	1	$z_1$	$z_2$	$z_3$	$z_1^2$	$z_2^2$	$z_3^2$	$\dots$
$\dot{z}_1$	1							
$\dot{z}_2$								
$\dot{z}_3$								

	1	$z_1$	$z_2$	$z_3$	$z_1^2$	$z_2^2$	$z_3^2$	$\dots$
$\dot{z}_1$	1							
$\dot{z}_2$								
$\dot{z}_3$								

## Dynamics



W

Discovery Models &  
Coordinates Simultaneously