Deep Learning for Universal Linear Embeddings of Nonlinear Dynamics

IPAM 2019

Operator Theoretic Methods in Dynamic Data Analysis and Control

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Bernard Koopman 1931

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

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

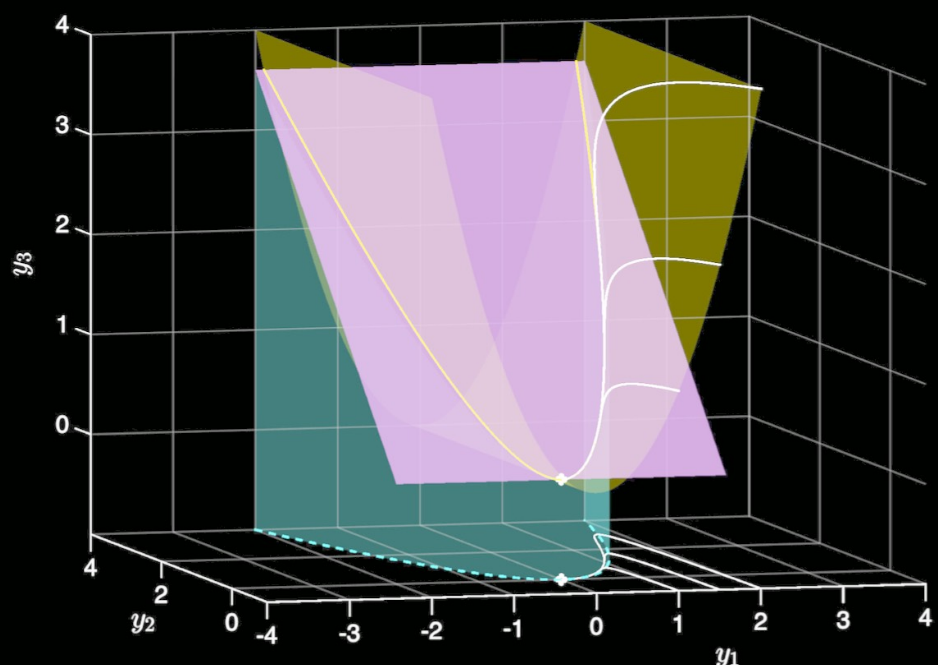
where $\mathbf{x} \in \mathbb{R}^n$ *is in a state space* $\mathbf{x} \in \mathscr{M}$. *The Koopman operator* $\mathscr{K}$ *acts on a set of scalar observable variables* g_j *which comprise the vector* $\mathbf{g} : \mathscr{M} \to \mathbb{C}$ *so that*

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

Mezic (2004)
Coifman, Kevrekidis, co-workers - Diffusion Maps
Williams et al - EDMD

Koopman Invariant Subspaces

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



Brunton, Proctor & Kutz, PLOS ONE (2018)

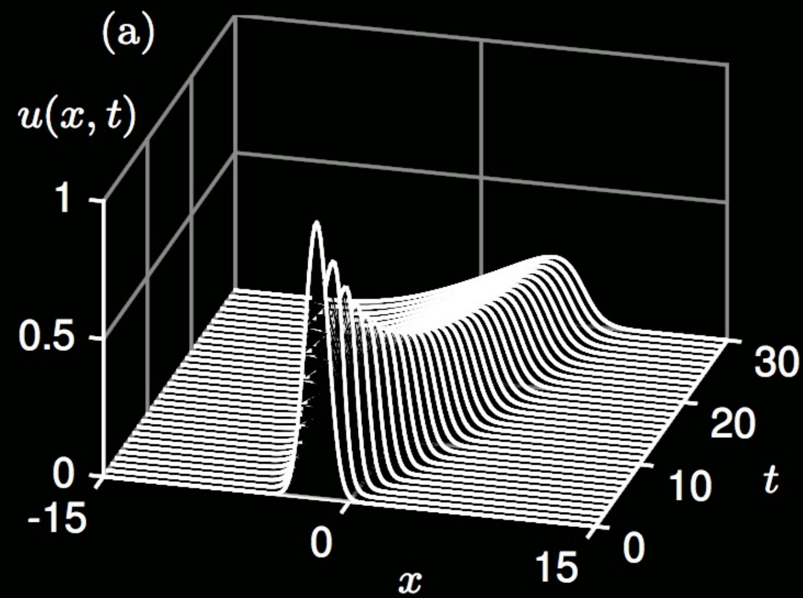
Burgers' Equation

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

Cole-Hopf

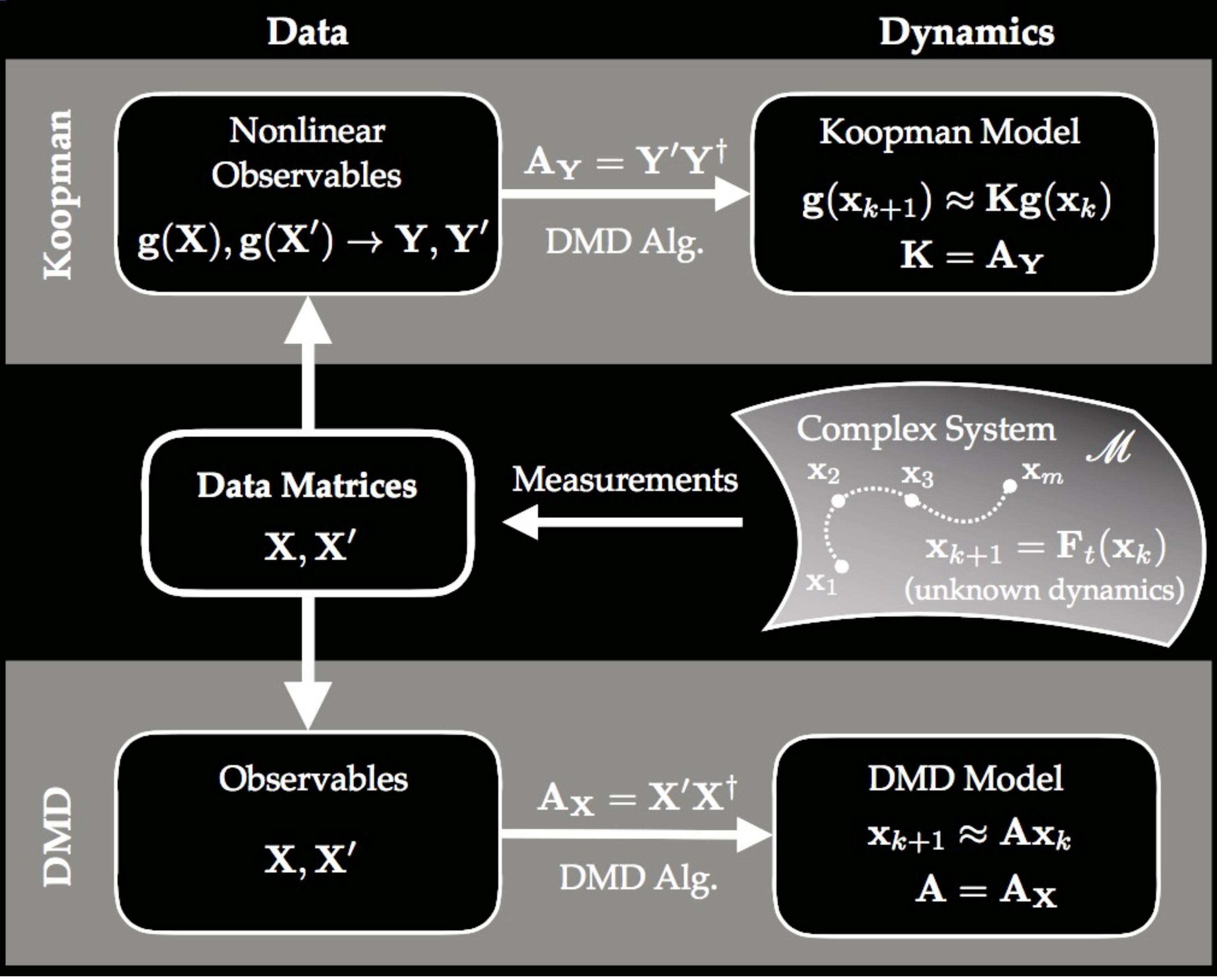
$$u = -2\epsilon v_x / v$$

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



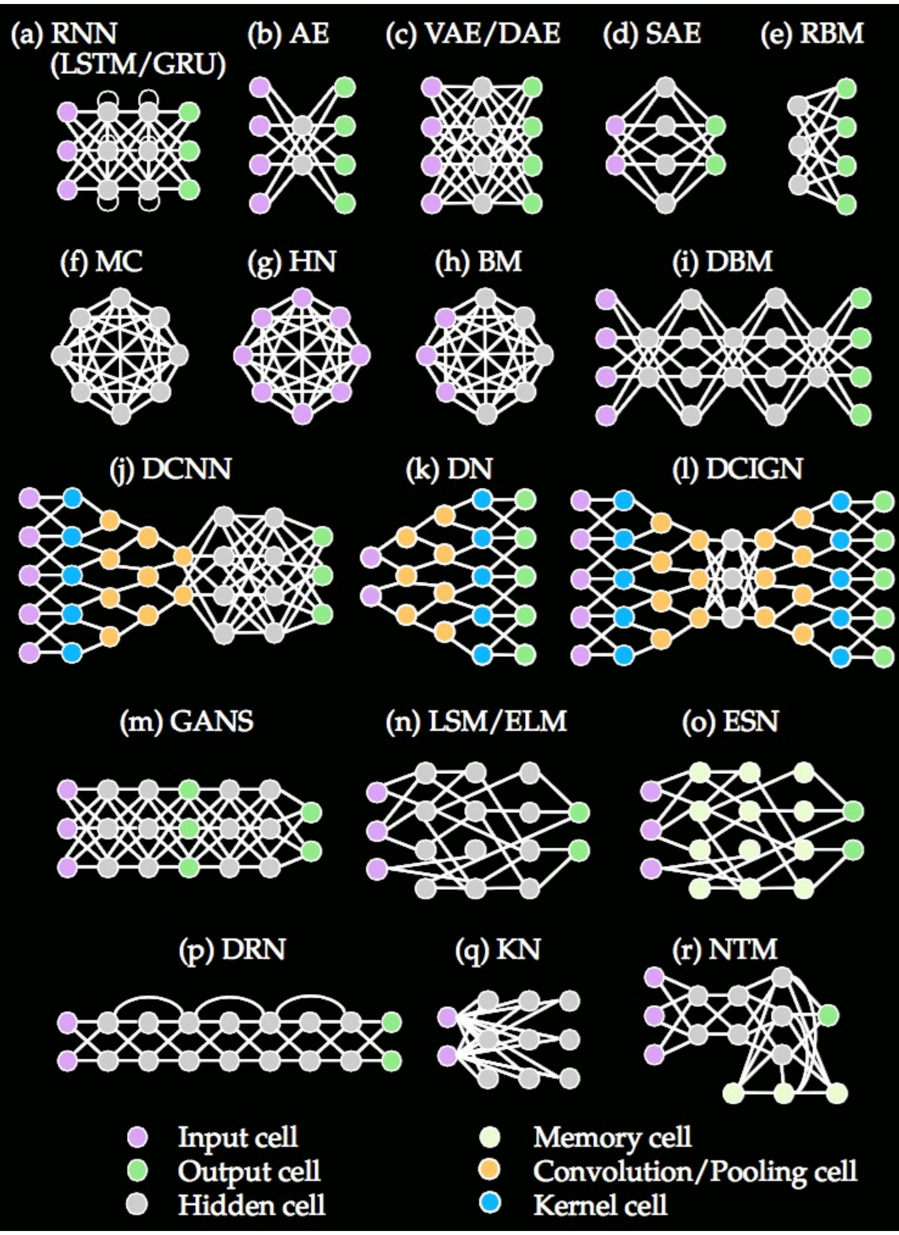
Kutz, Proctor & Brunton, Complexity (2018)

Koopman vs DMD: All about Observables!

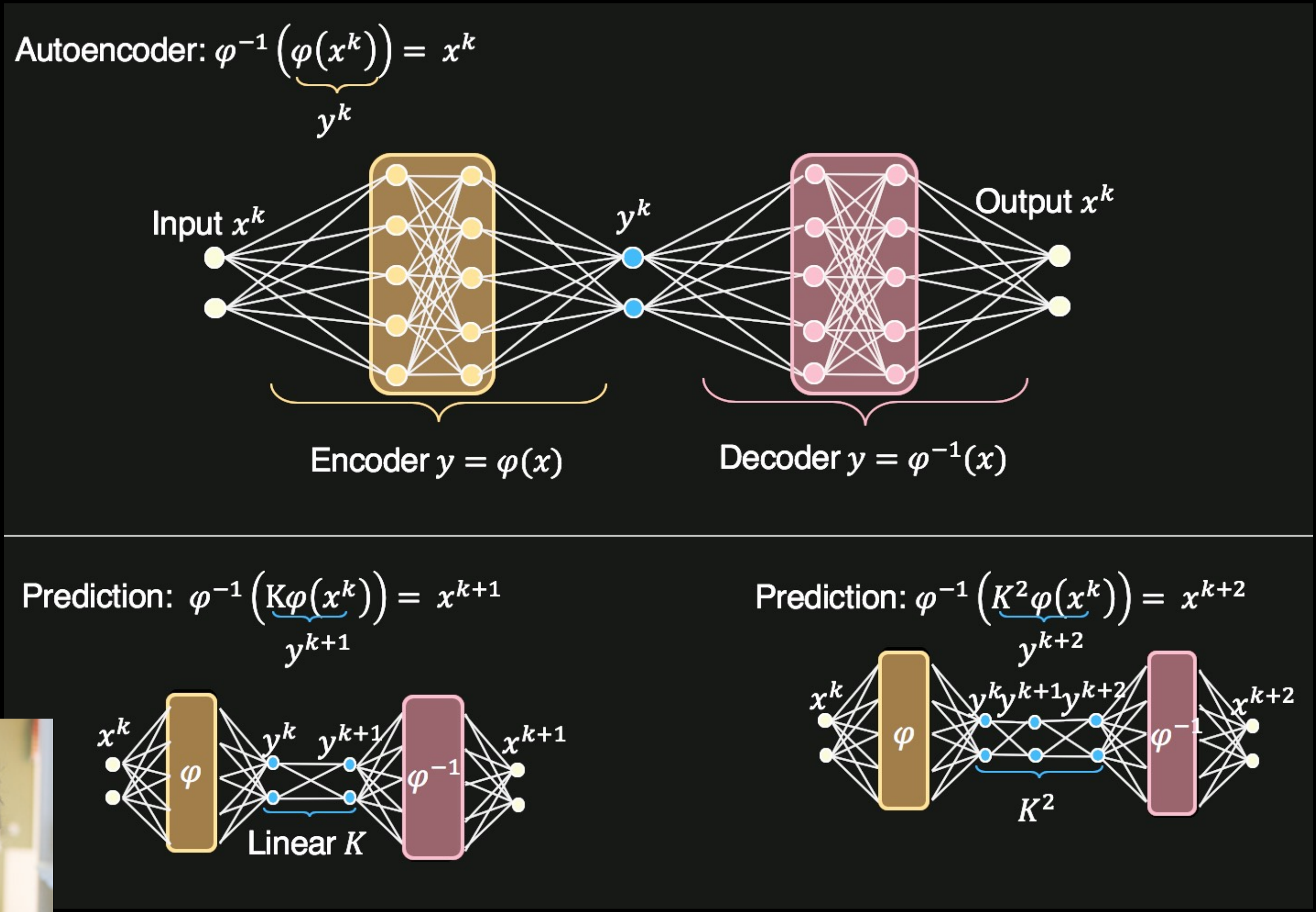


Neural Nets

NN Zoo


(a) RNN (LSTM/GRU)
(b) AE
(c) VAE/DAE
(d) SAE
(e) RBM
(f) MC
(g) HN
(h) BM
(i) DBM
(j) DCNN
(k) DN
(l) DCIGN
(m) GANS
(n) LSM/ELM
(o) ESN
(p) DRN
(q) KN
(r) NTM
Input cell
Output cell
Hidden cell
Memory cell
Convolution/Pooling cell
Kernel cell

NNs for Koopman Embedding



Bethany Lusch

Lusch et al. Nat. Comm (2018)

Failure!

(obviously)

Duffing Oscillator

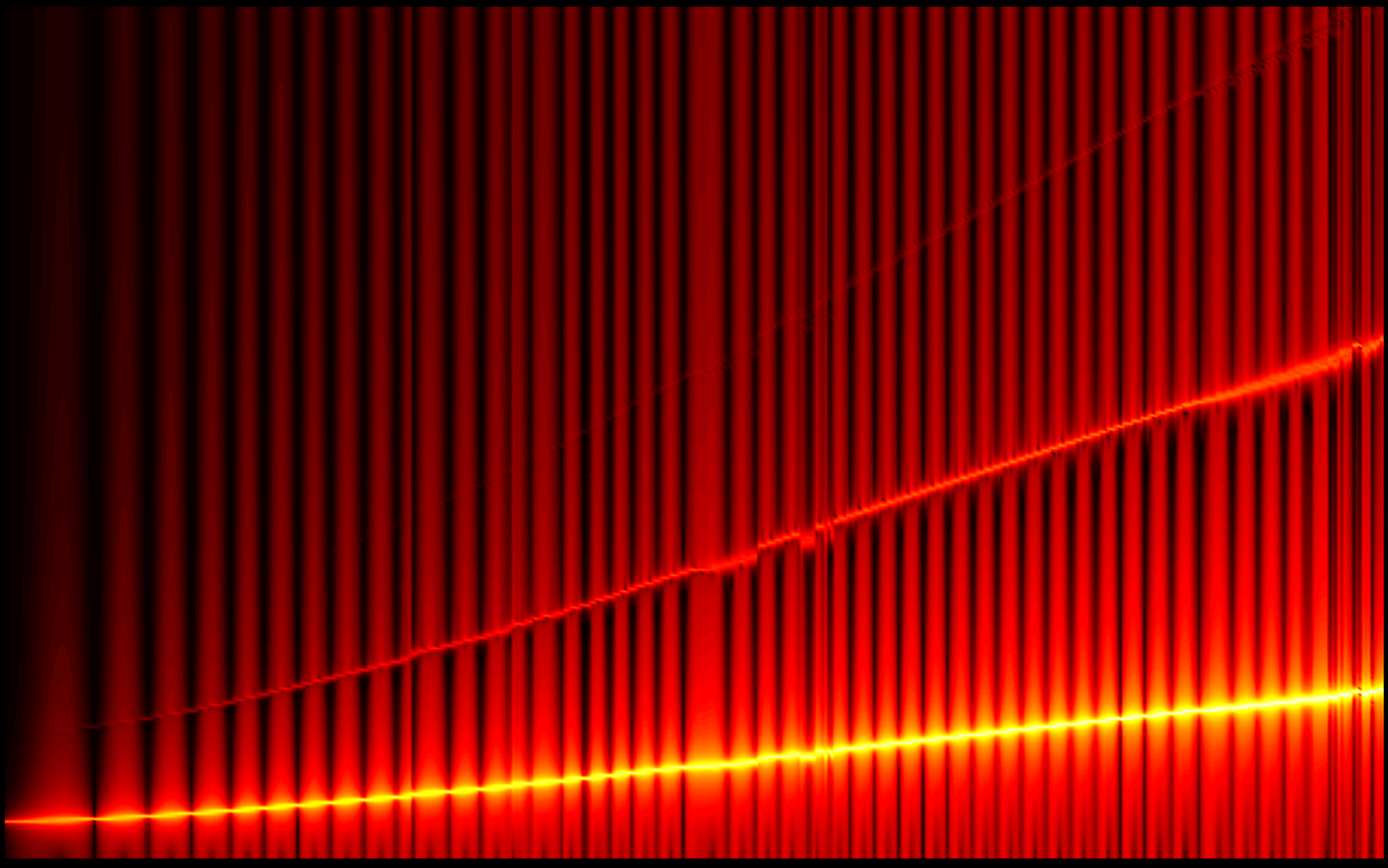
Poincare-Lindstedt Expansion: let $\tau = \omega t$ so that

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

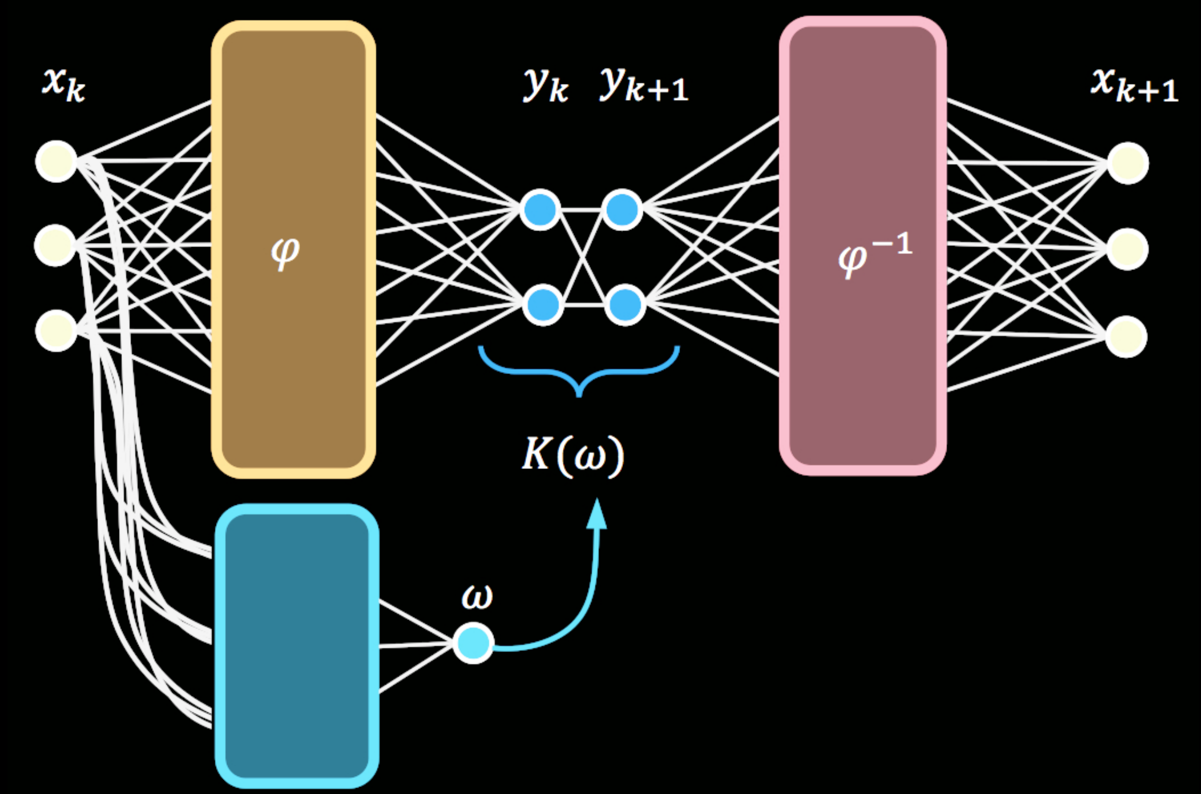
Nonlinearity: Shifts Frequencies + Generates Harmonics

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

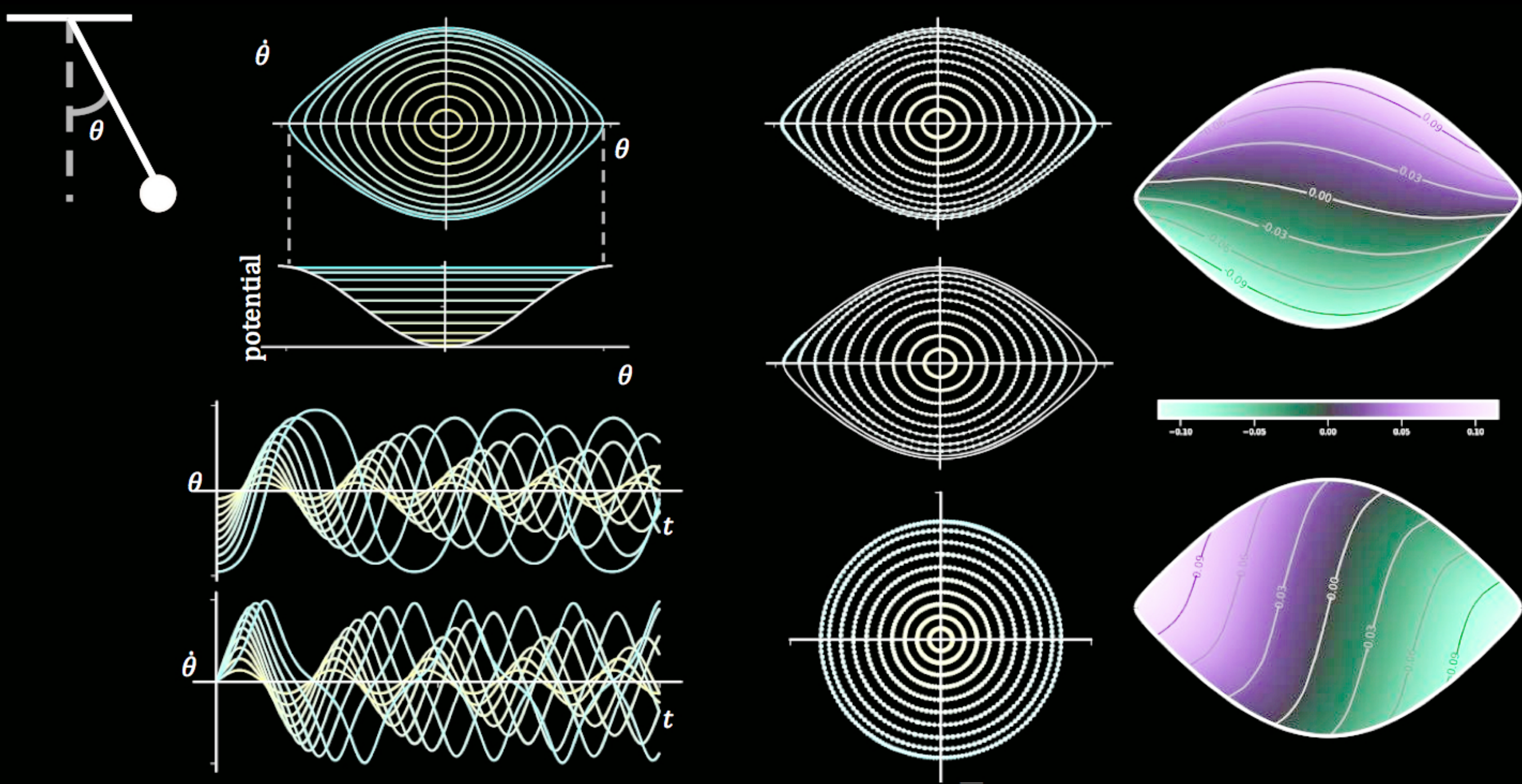
Spectrogram



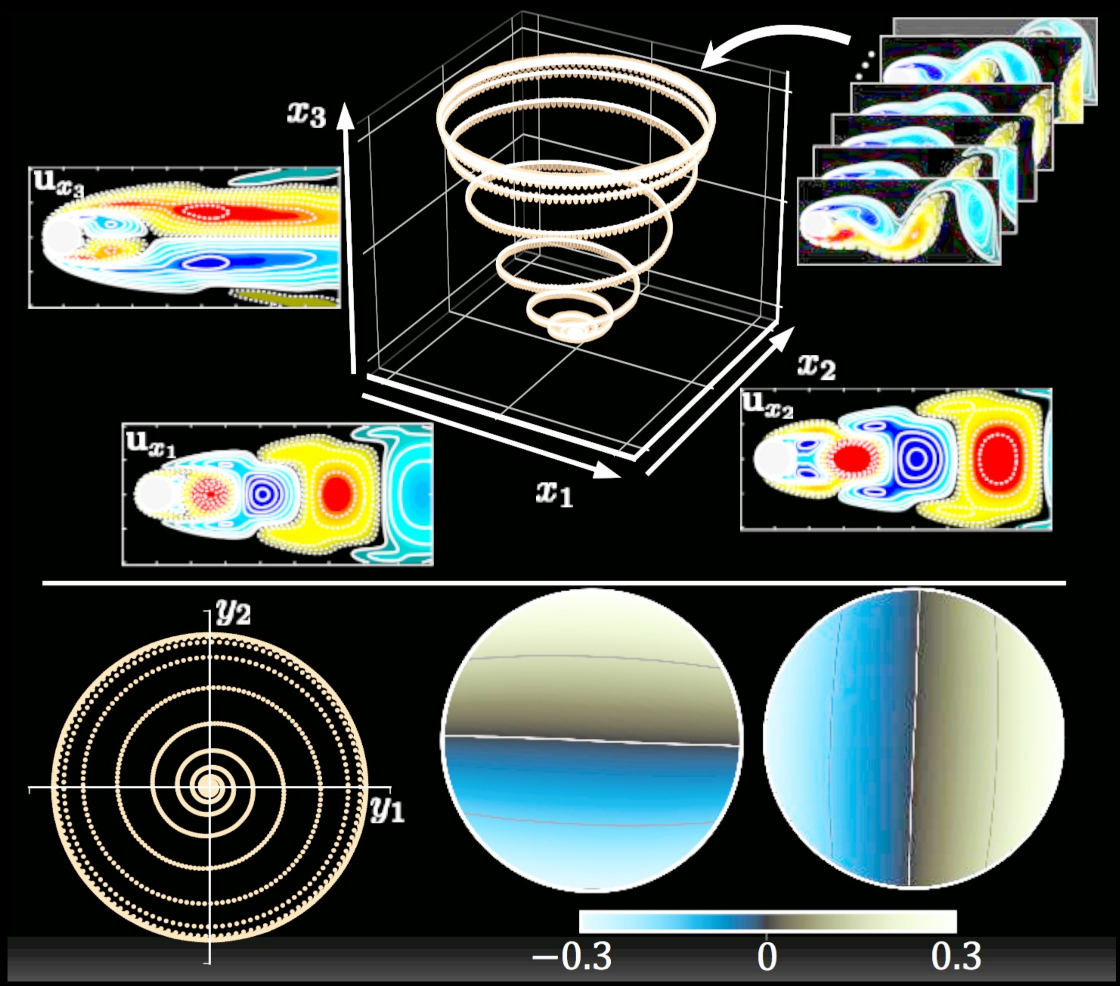
Handling the Continuous Spectra



The Pendulum



Flow Around a Cylinder



Relax Koopman

Sparse Identification of Nonlinear Dynamics (SINDy)

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

↓

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

Sparse Identification of Nonlinear Dynamics (SINDy)

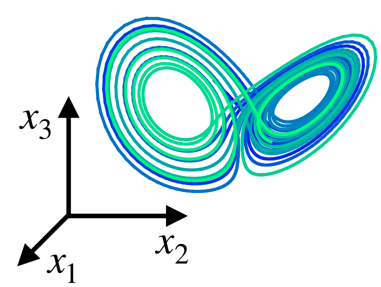
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t))$$

⬇

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

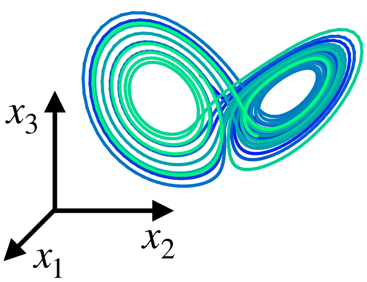
Example: Lorenz

$$\dot{x}_1 = \sigma(x_2 - x_1)$$
$$\dot{x}_2 = x_1(\rho - x_3) - x_2$$
$$\dot{x}_3 = x_1 x_2 - \beta x_3$$



Sparse Identification of Nonlinear Dynamics (SINDy)

True System



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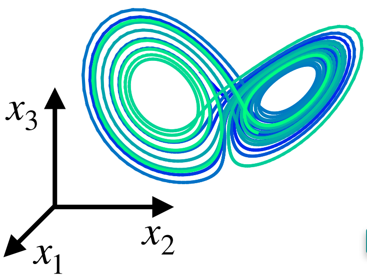
Sparse Identification of Nonlinear Dynamics (SINDy)

True System

SINDy fitting



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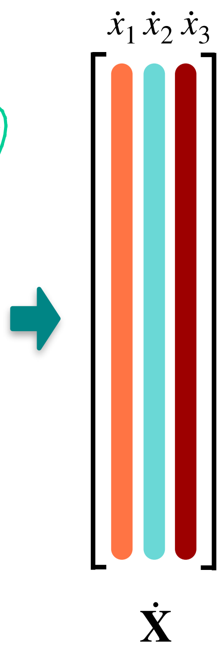

Sparse Identification of Nonlinear Dynamics (SINDy)

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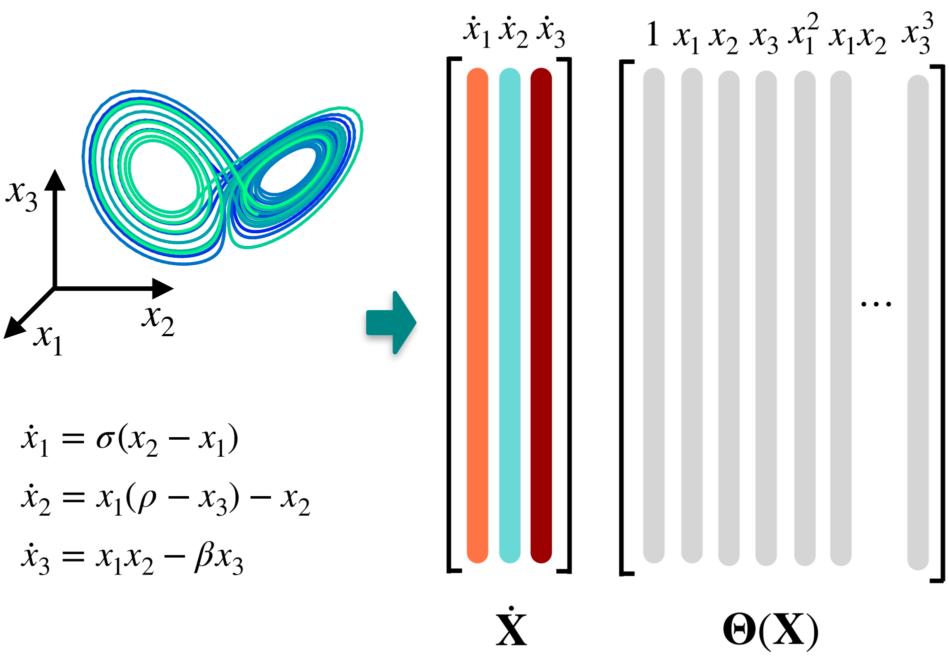
SINDy fitting



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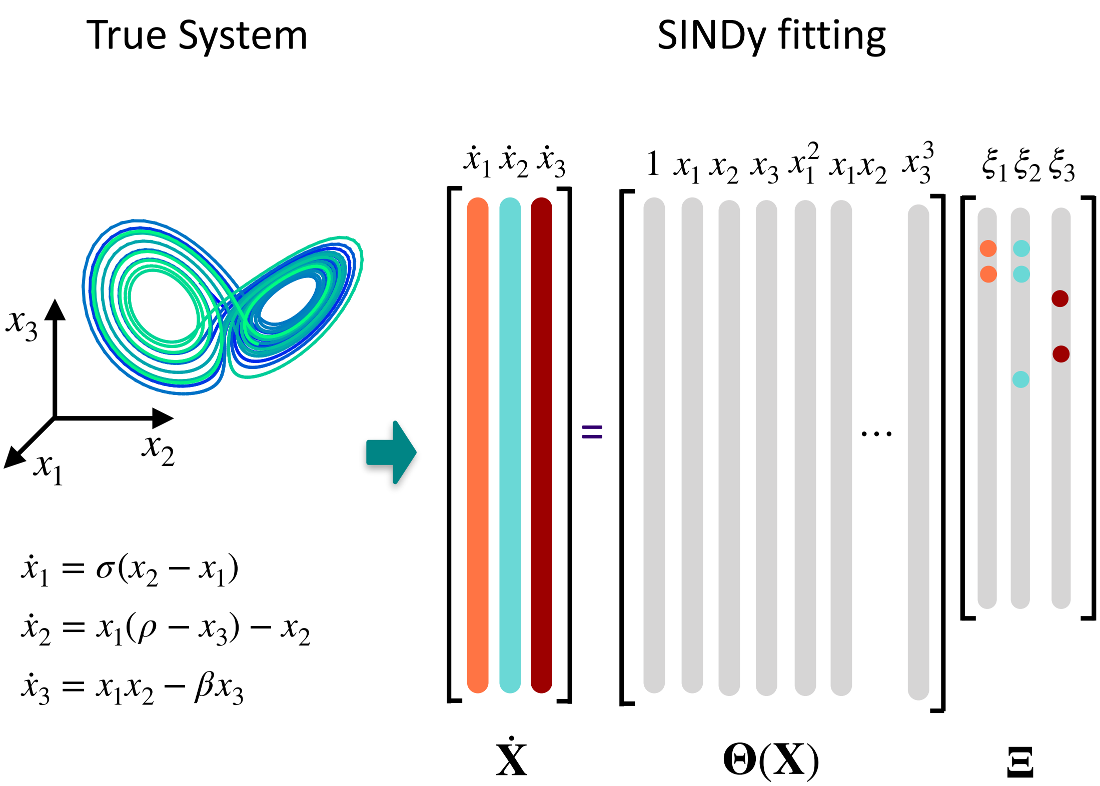
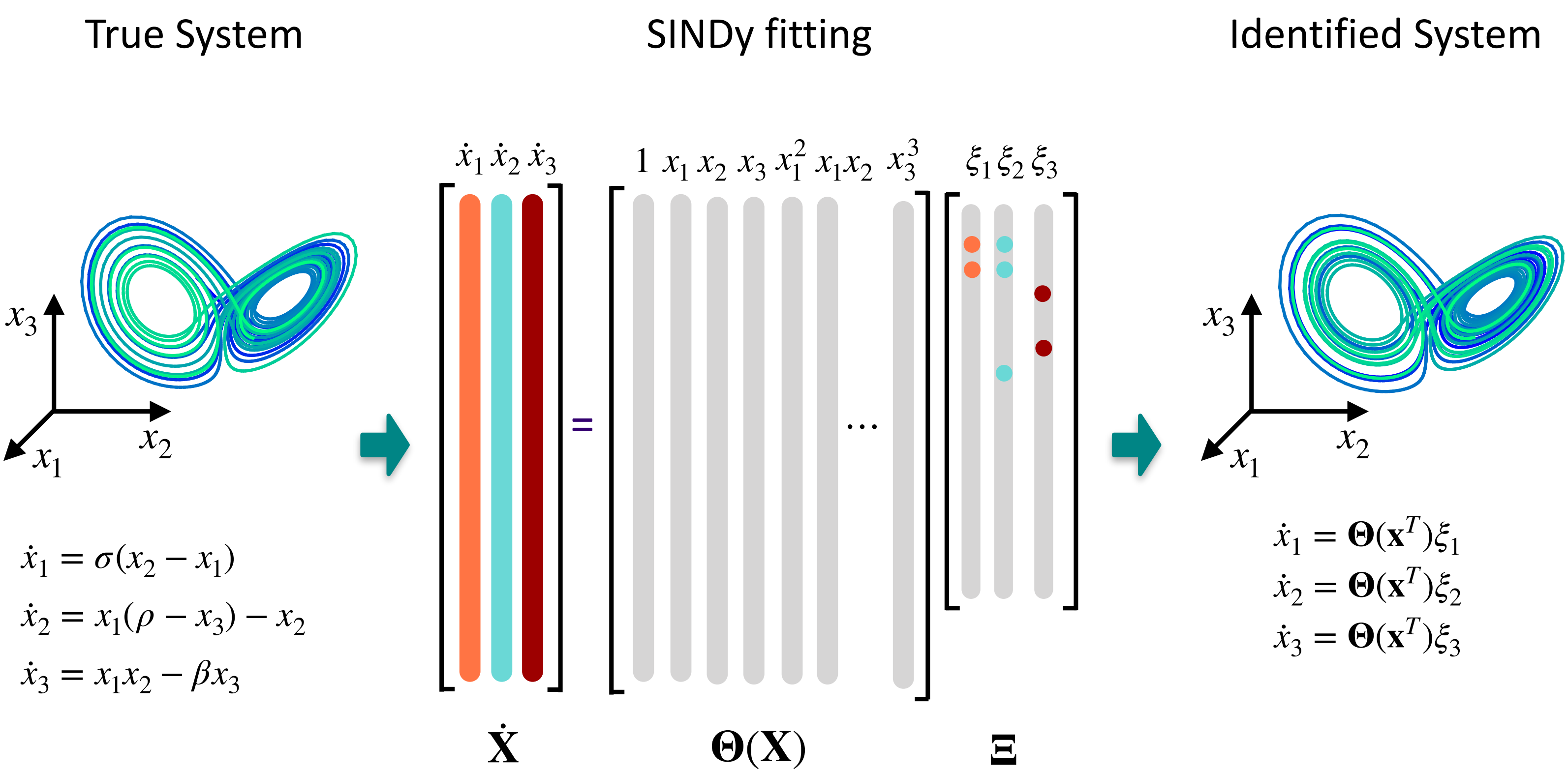
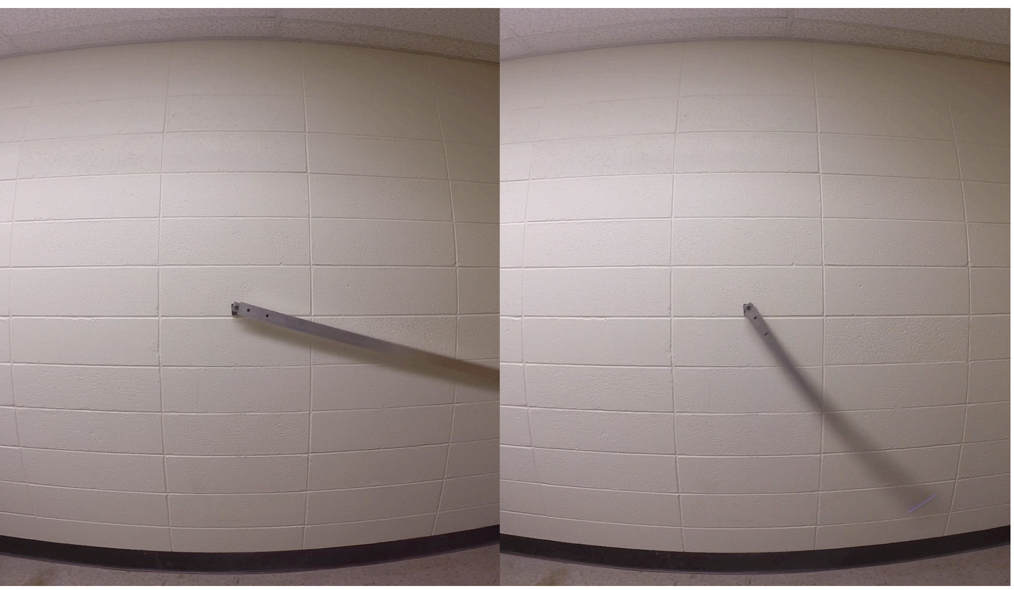
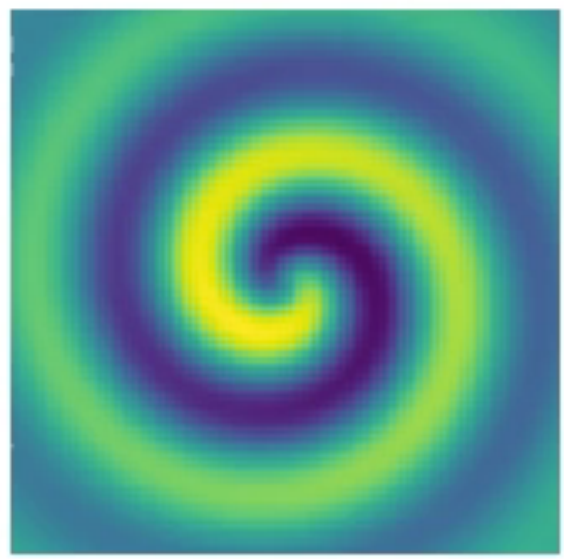


Sparse Identification of Nonlinear Dynamics (SINDy)

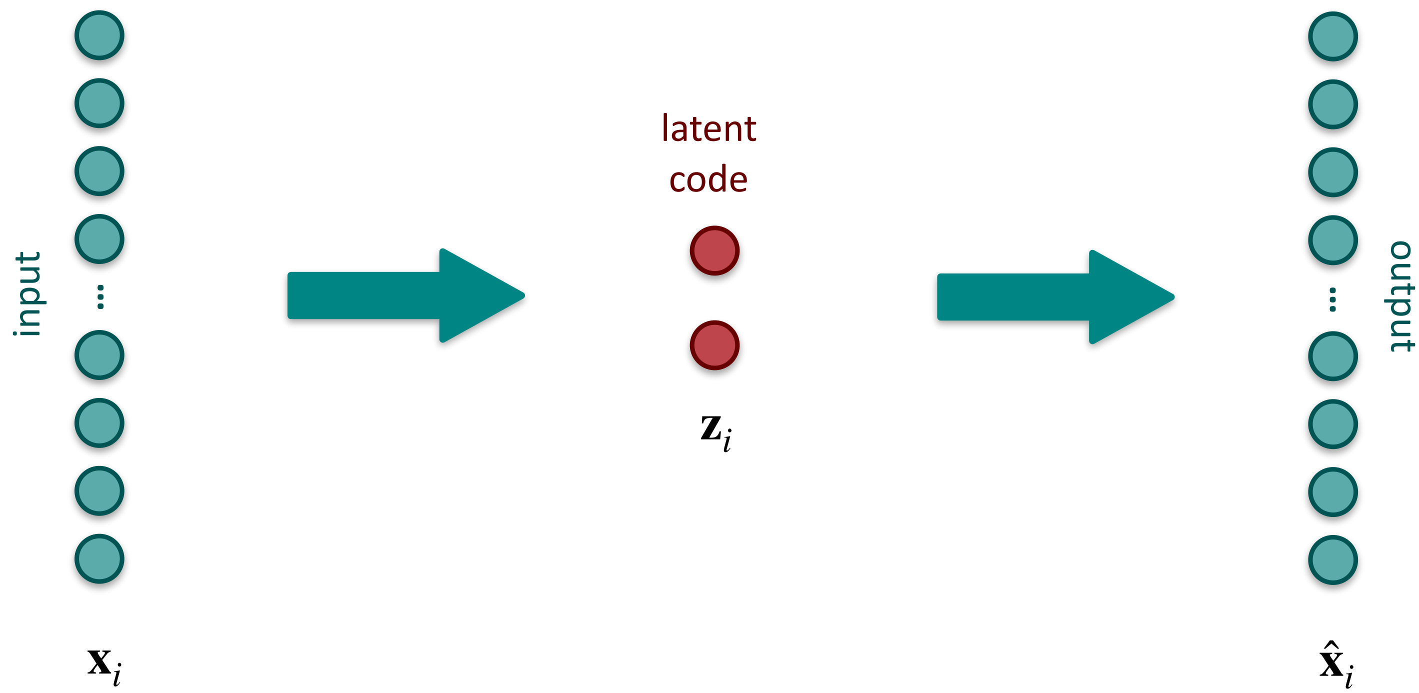


What if we don’t know the right coordinates?



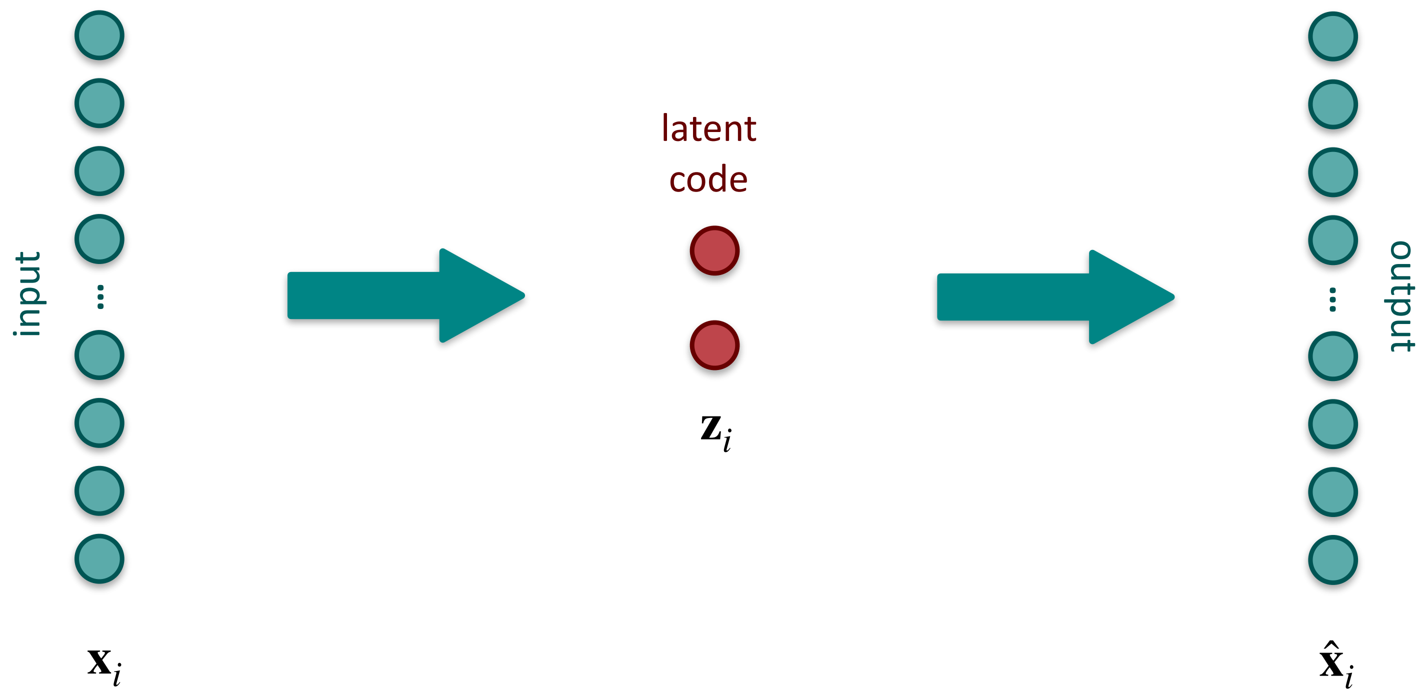


Autoencoder



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

Autoencoder



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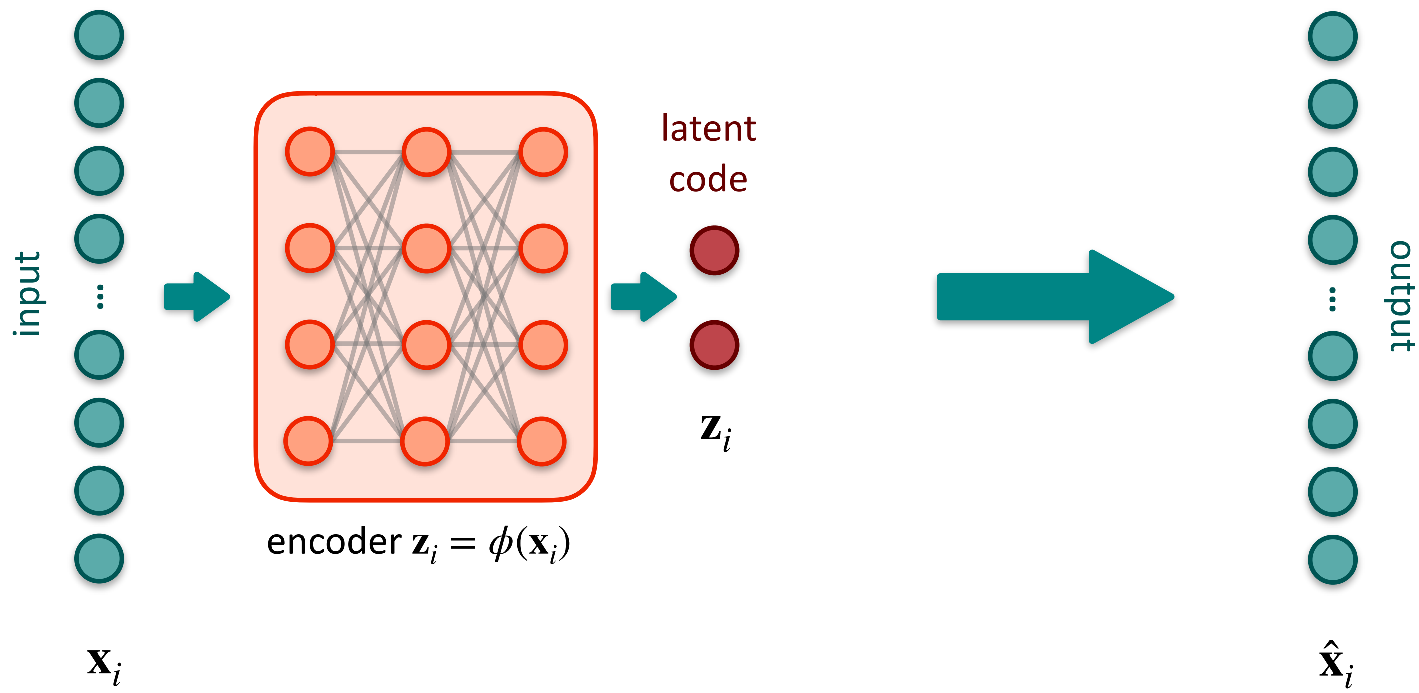
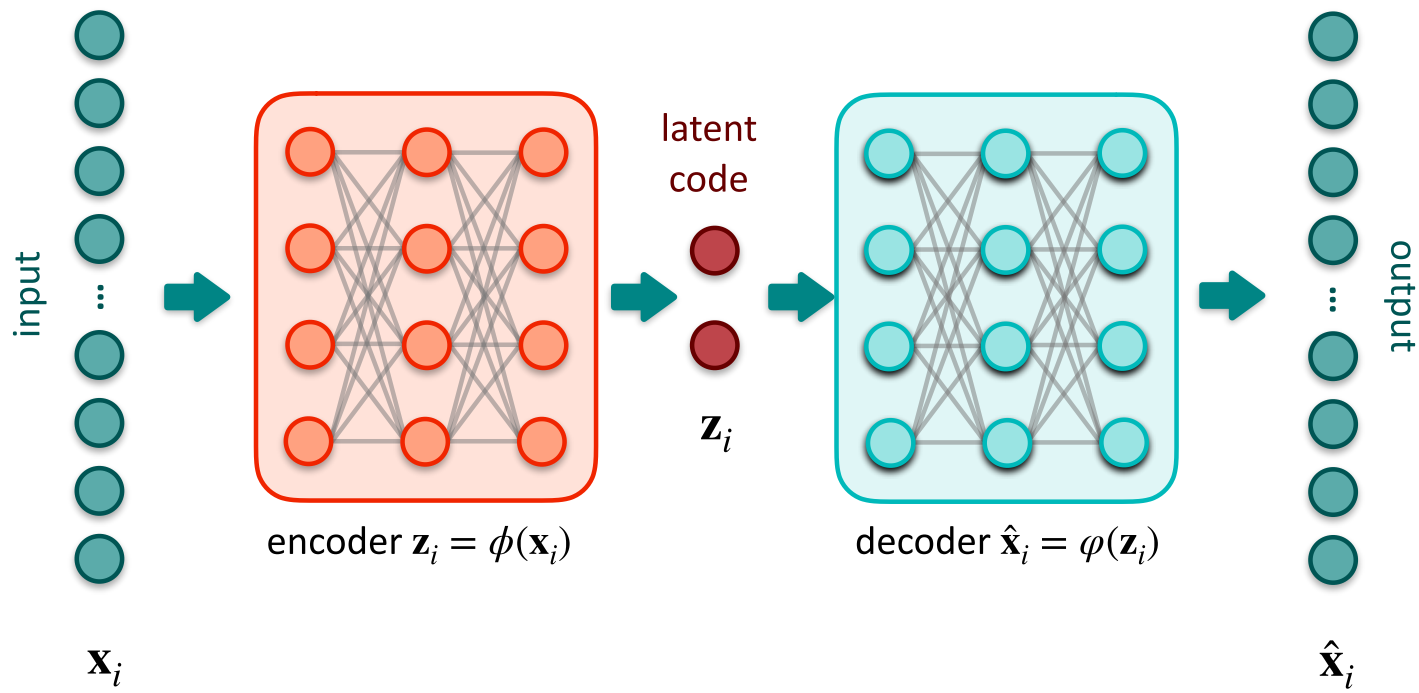


loss function: $\frac{1}{N}\sum_{i=1}^{N} \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$

Autoencoder



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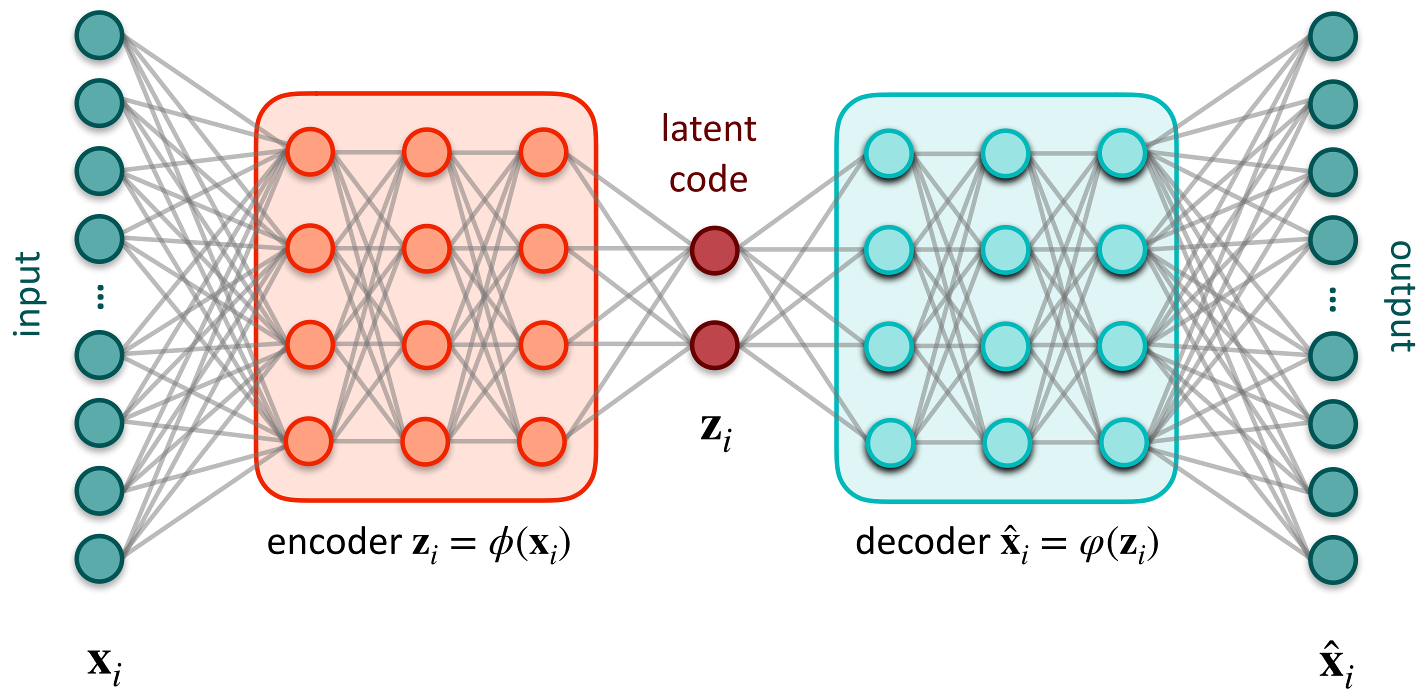
Autoencoder



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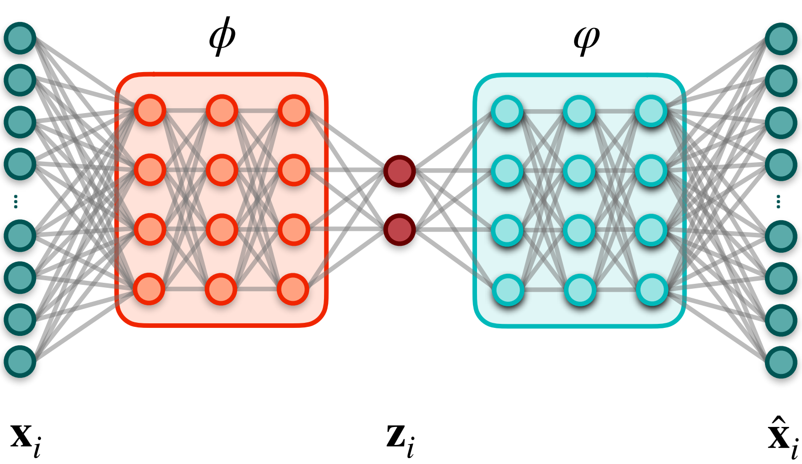
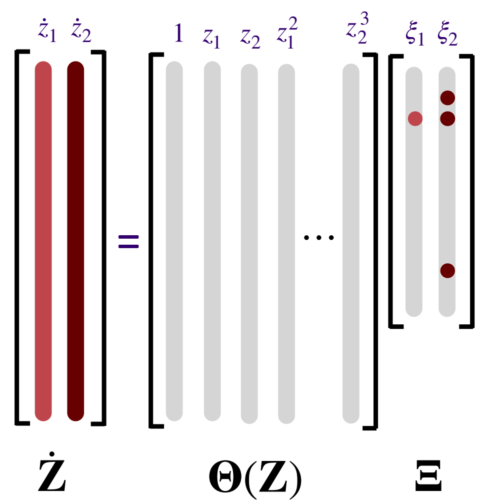
Autoencoder + SINDy

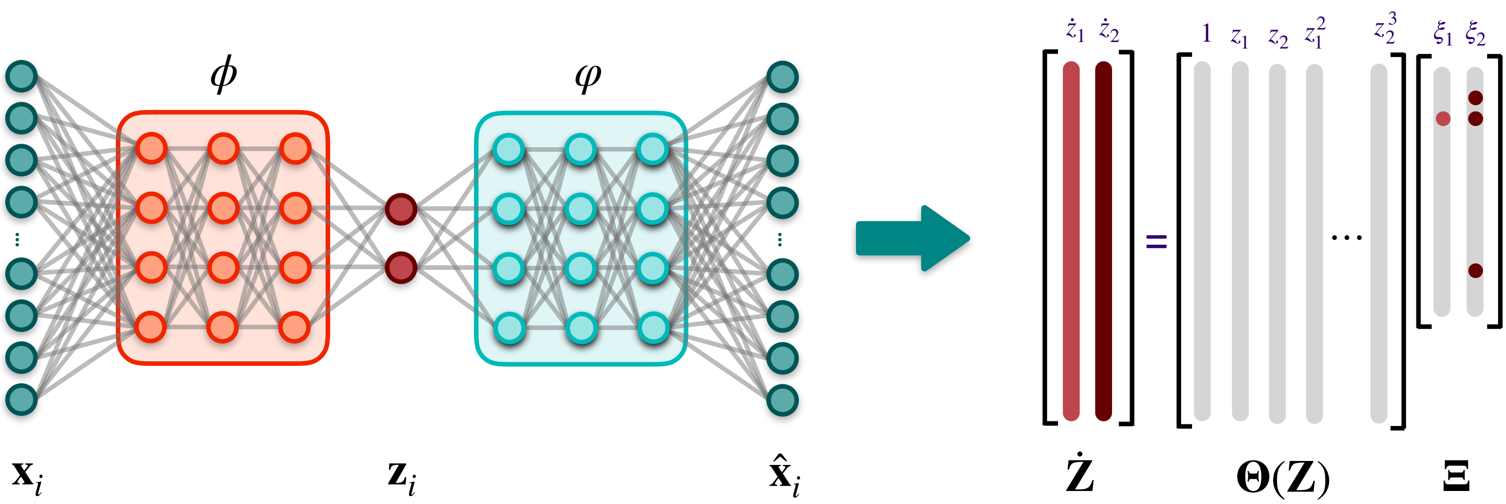




loss: $$\frac{1}{N}\sum_{i=1}^{N} \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2^2$$

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

Autoencoder + SINDy



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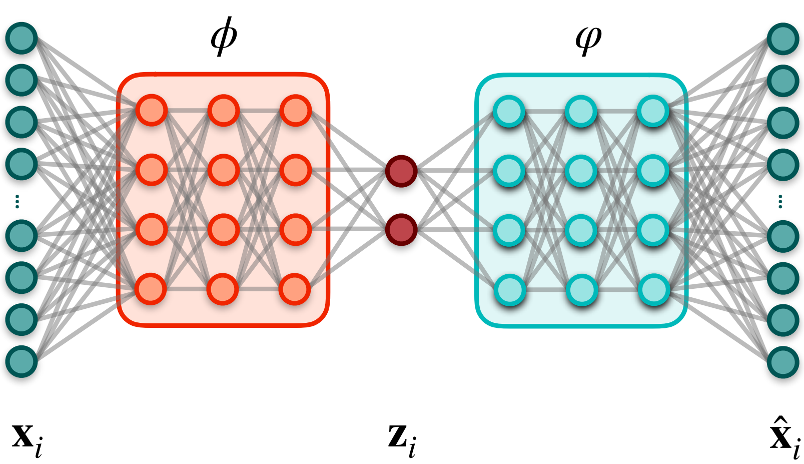

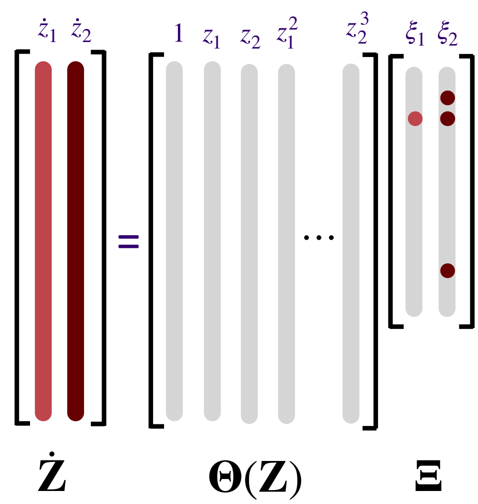

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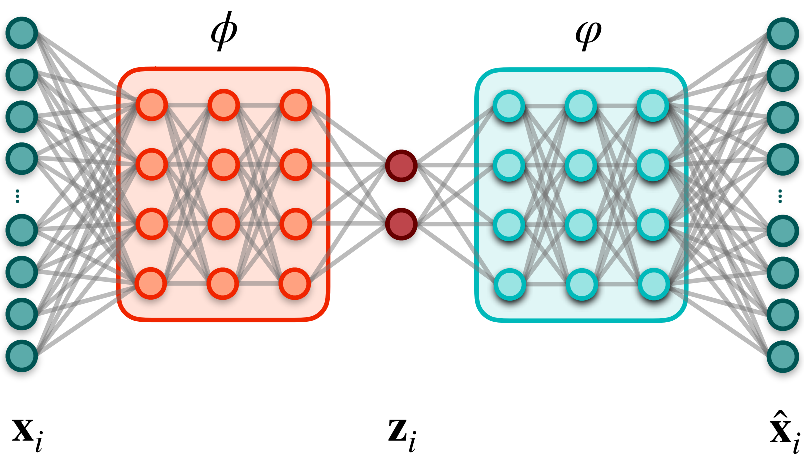
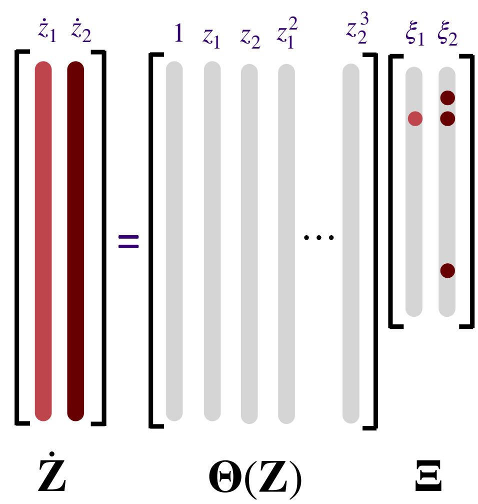
Autoencoder + SINDy



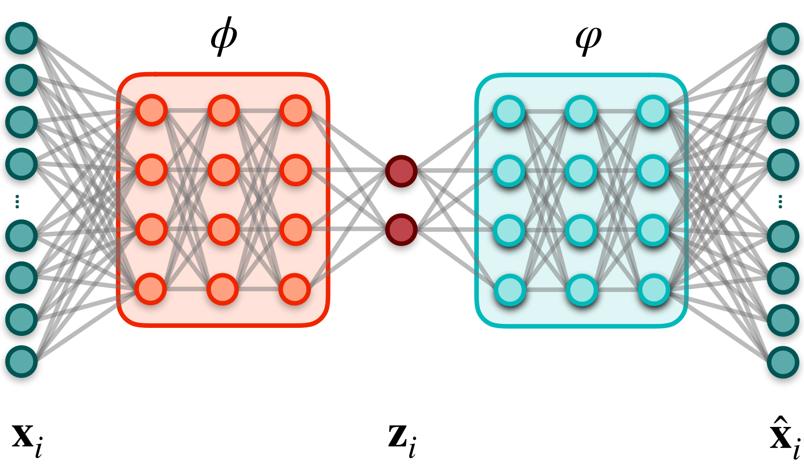


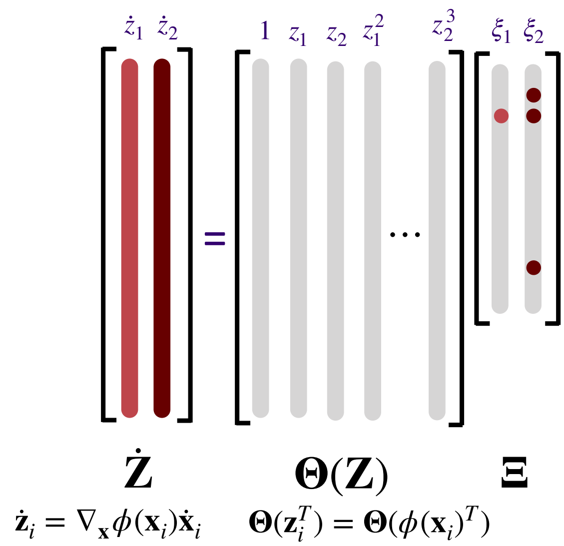
$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}}\phi(\mathbf{x}_i)\dot{\mathbf{x}}_i$

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

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

Autoencoder + SINDy





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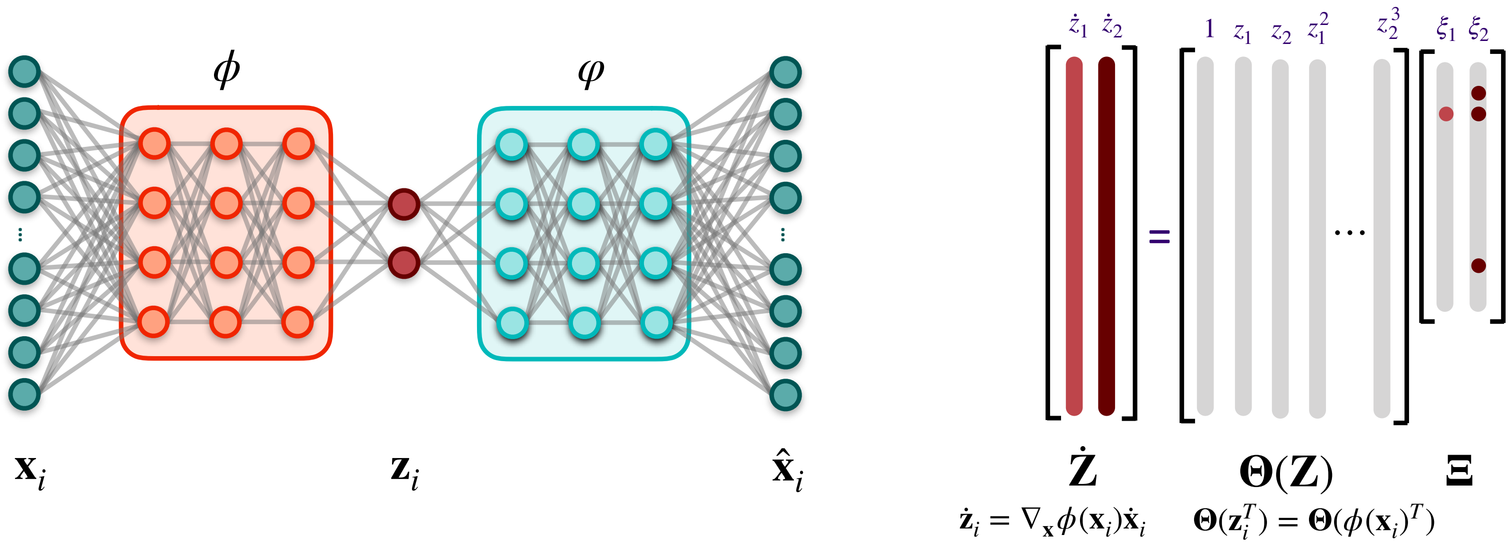
Autoencoder + SINDy

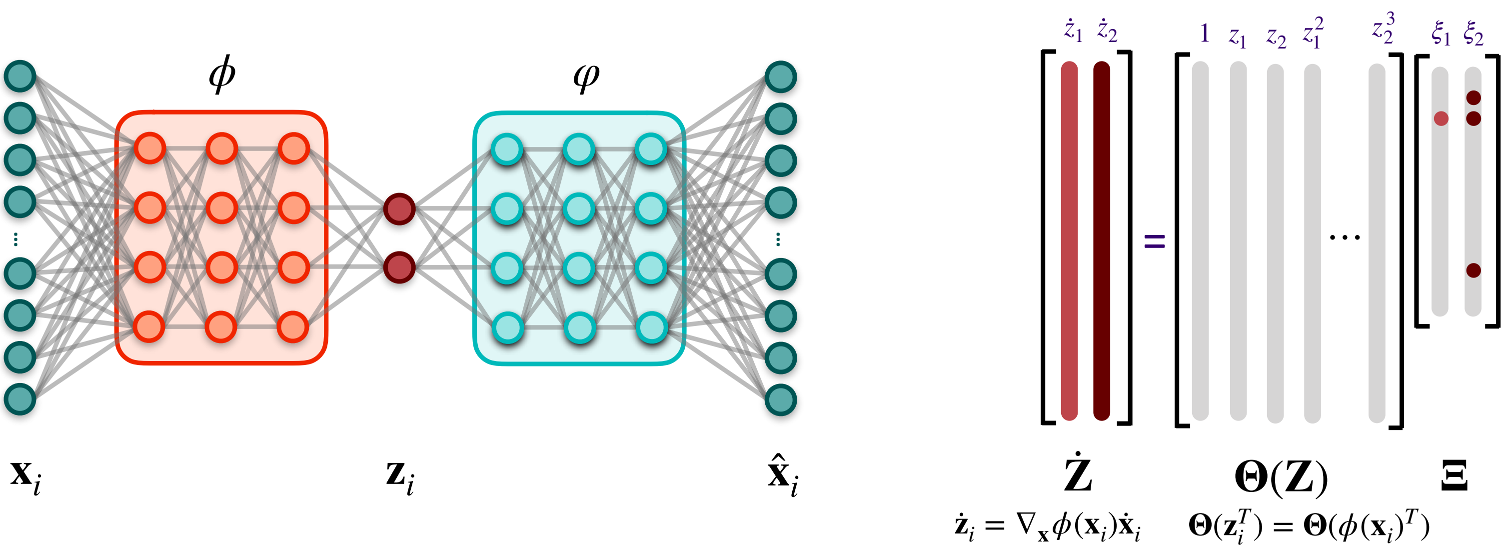


loss: $$\lambda_1 \frac{1}{N}\sum_{i=1}^{N} \|\mathbf{x}_i - \varphi(\phi(\mathbf{x}_i))\|_2^2 \; + \; \lambda_2 \frac{1}{N}\sum_{i=1}^{N} \|\nabla_{\mathbf{x}}\phi(\mathbf{x}_i)\dot{\mathbf{x}}_i - \boldsymbol{\Theta}(\phi(\mathbf{x}_i)^T)\boldsymbol{\Xi}\|_2^2$$

autoencoder component

SINDy component

Autoencoder + SINDy



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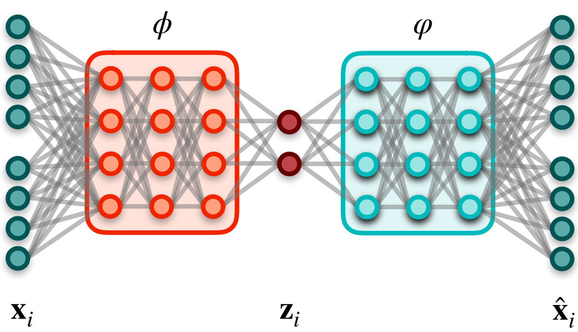
autoencoder component

SINDy component

Autoencoder + SINDy



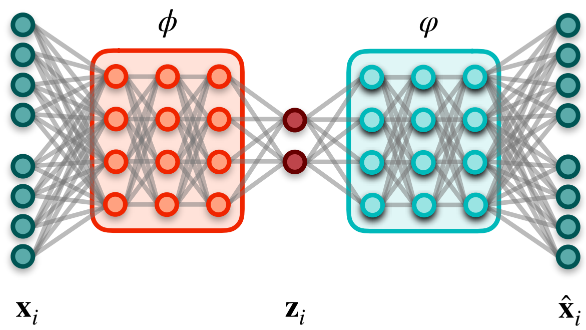
loss:

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

L_1 L_2 L_3

> ***Issue:*** training shrinks norm of **z** to minimize loss function

Autoencoder + SINDy



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L_1 L_2 L_3

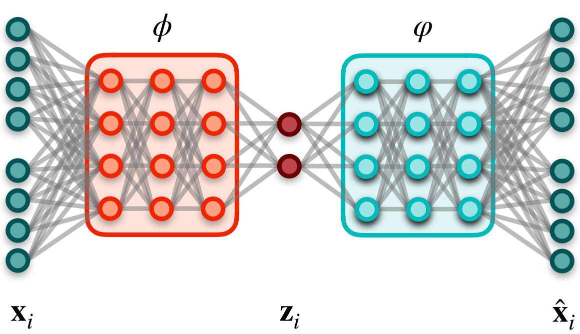
> ***Issue:*** training shrinks norm of **z** to minimize loss function

> ***Solution:*** use the following to enforce SINDy loss

new L_2 :

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

Autoencoder + SINDy



loss:

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> New loss function:

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

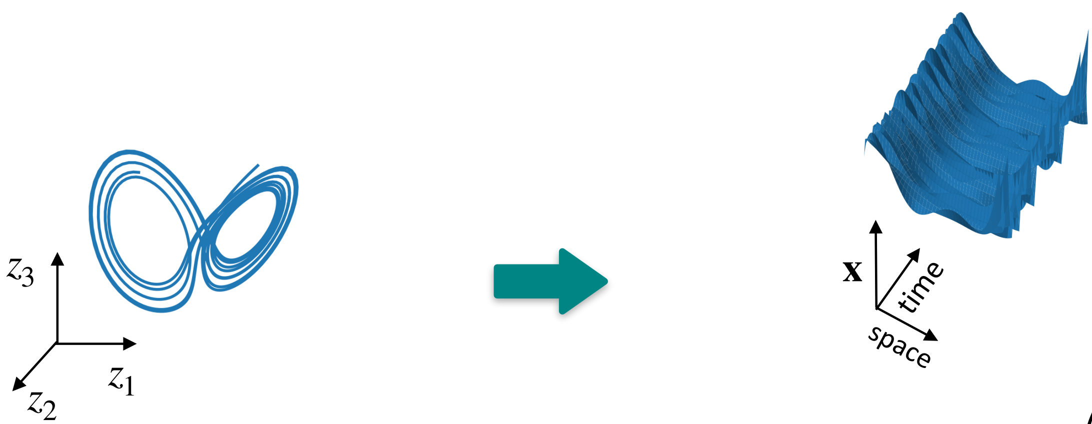
Achieving sparsity

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

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

- Instead combine L1 penalty with sequential thresholding

Example problem



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

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

$$\mathbf{A}, \mathbf{B} \in \mathbb{R}^{128\times3}$$

Example problem

Lorenz model

Equations

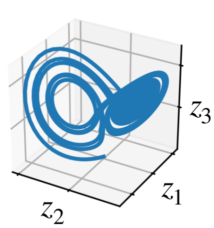
$$\dot{z}_1 = -10z_1 + 10z_2$$

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

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

Coefficient Matrix Ξ

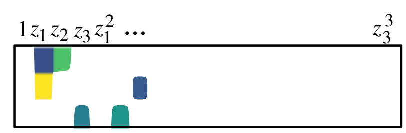
Dynamics



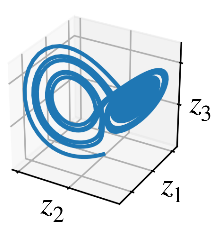
Example problem

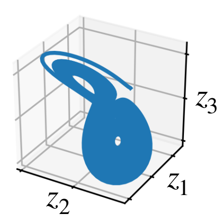
	Lorenz model	Discovered model	Discovered model (transformed)
Equations	$\dot{z}_1 = -10z_1 + 10z_2$	$\dot{z}_1 = -8.5z_2z_3$	$\dot{z}_1 = -10.2z_1 + 8.8z_2$
	$\dot{z}_2 = 28z_1 - z_2 - z_1z_3$	$\dot{z}_2 = 9.2 - 2.9z_2 + 1.1z_1z_3$	$\dot{z}_2 = 26.7z_1 - 8.5z_1z_3$
	$\dot{z}_3 = -2.7z_3 + z_1z_2$	$\dot{z}_3 = -8.8z_1 - 10.3z_3$	$\dot{z}_3 = -2.9z_3 + 1.1z_2$

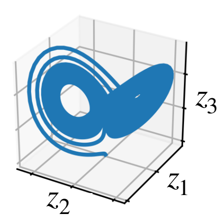
Coefficient Matrix Ξ



Dynamics







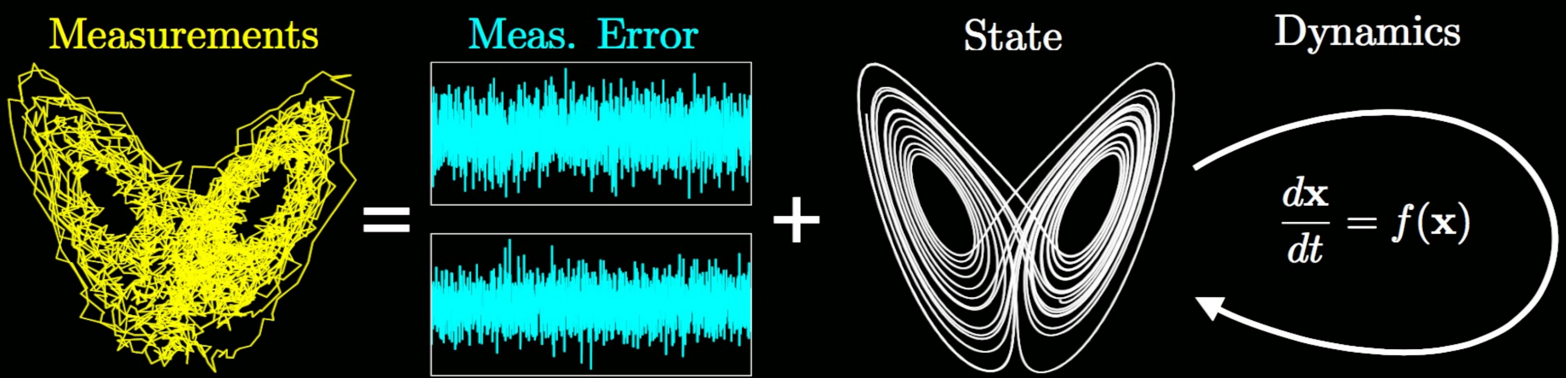
Realities of Life

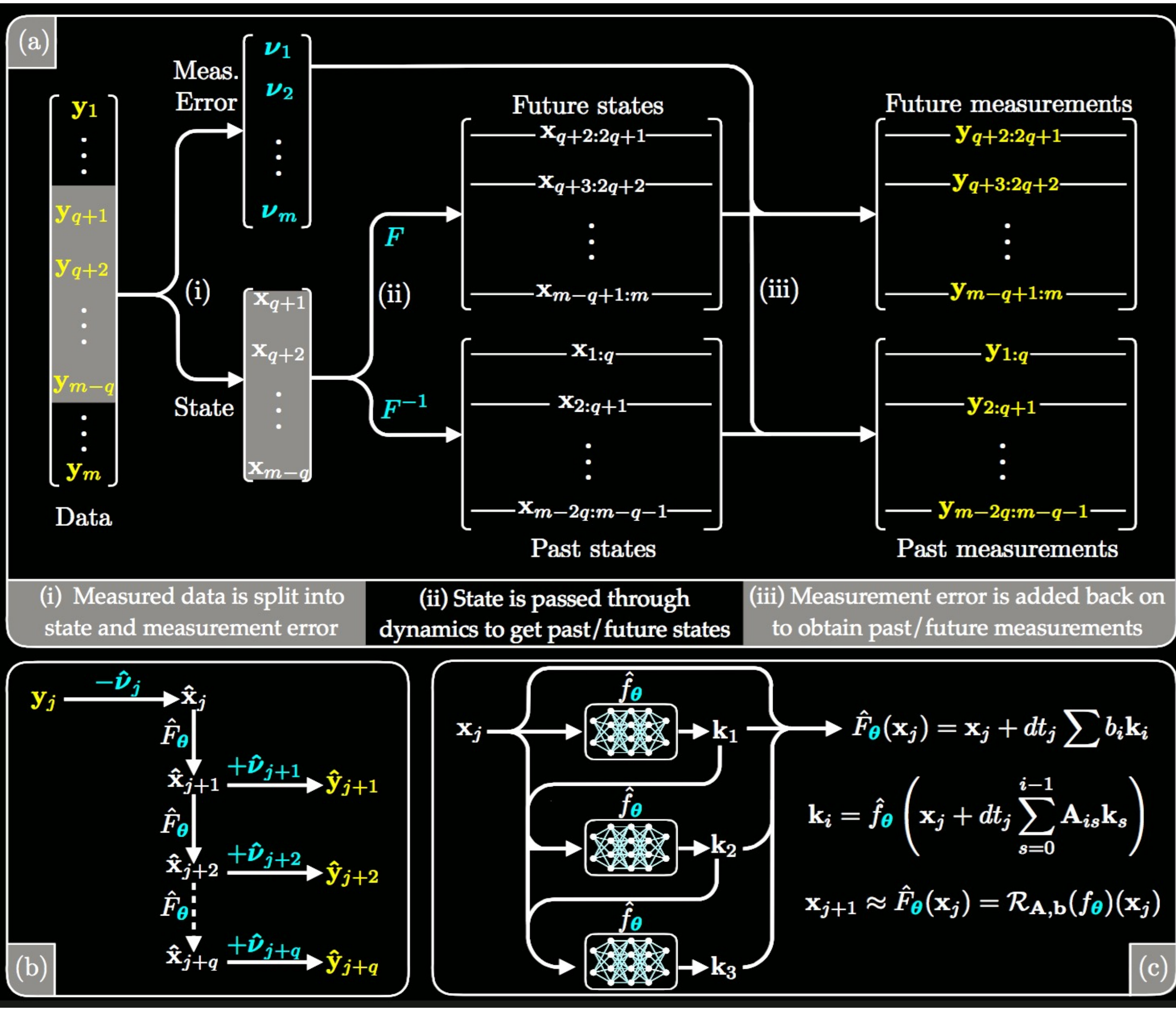
&

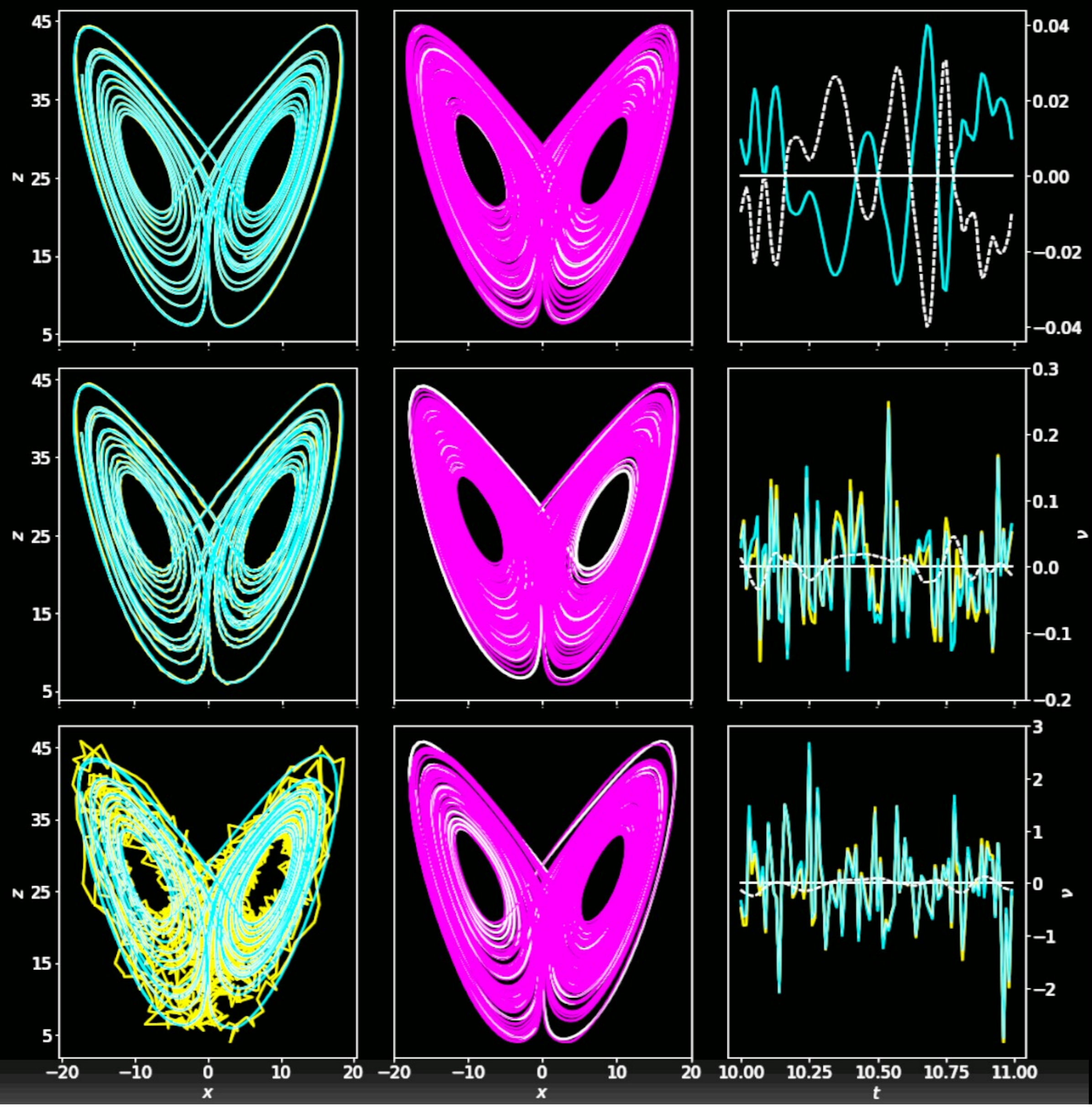
NN Magic

Noise

Sam Rudy


Measurements
Meas. Error
State
Dynamics
$\frac{d\mathbf{x}}{dt} = f(\mathbf{x})$


(a)
Meas.
Error
ν_1
ν_2
ν_m
y_1
y_{q+1}
y_{q+2}
y_{m-q}
y_m
Data
(i)
State
x_{q+1}
x_{q+2}
x_{m-q}
(ii)
F
F^{-1}
Future states
$x_{q+2:2q+1}$
$x_{q+3:2q+2}$
$x_{m-q+1:m}$
$x_{1:q}$
$x_{2:q+1}$
$x_{m-2q:m-q-1}$
Past states
(iii)
Future measurements
$y_{q+2:2q+1}$
$y_{q+3:2q+2}$
$y_{m-q+1:m}$
$y_{1:q}$
$y_{2:q+1}$
$y_{m-2q:m-q-1}$
Past measurements
(i) Measured data is split into state and measurement error
(ii) State is passed through dynamics to get past/future states
(iii) Measurement error is added back on to obtain past/future measurements
(b)
y_j $-\hat{\nu}_j$ $\hat{x}_j$
$\hat{F}_\theta$
$\hat{x}_{j+1}$ $+\hat{\nu}_{j+1}$ $\hat{y}_{j+1}$
$\hat{x}_{j+2}$ $+\hat{\nu}_{j+2}$ $\hat{y}_{j+2}$
$\hat{x}_{j+q}$ $+\hat{\nu}_{j+q}$ $\hat{y}_{j+q}$
(c)
x_j
$\hat{f}_\theta$
k_1
k_2
k_3
$\hat{F}_\theta(x_j) = x_j + dt_j \sum b_i k_i$
$k_i = \hat{f}_\theta \left(x_j + dt_j \sum_{s=0}^{i-1} A_{is} k_s \right)$
$x_{j+1} \approx \hat{F}_\theta(x_j) = \mathcal{R}_{A,b}(f_\theta)(x_j)$

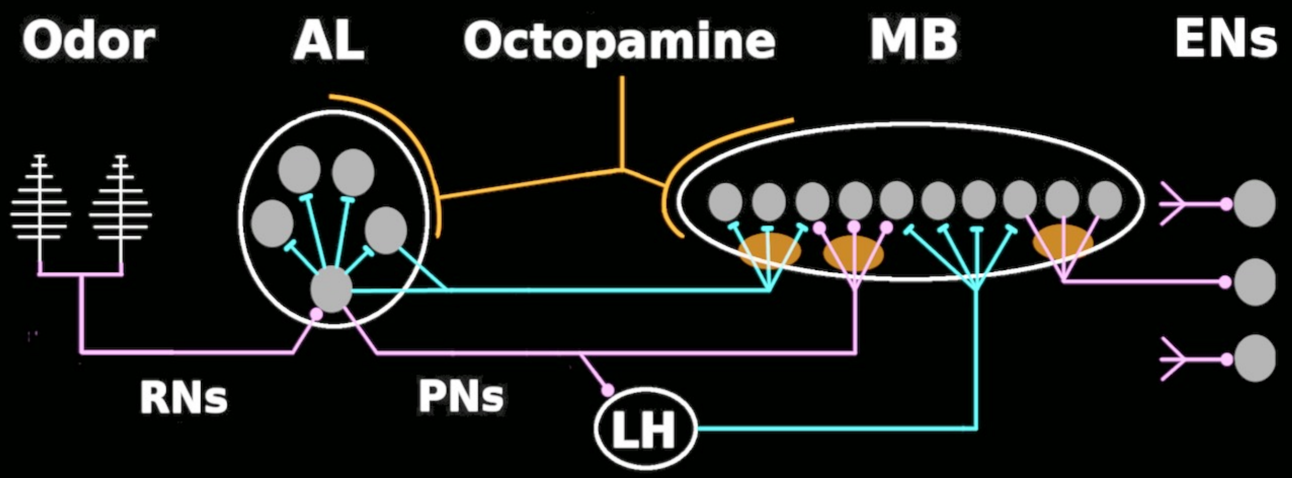


45
35
z 25
15
5
0.04
0.02
0.00
−0.02
−0.04
0.3
0.2
0.1
0.0
−0.1
−0.2
y
3
2
1
0
−1
−2
−20 −10 0 10 20
x
10.00 10.25 10.50 10.75 11.00
t

Fast Learning

Charles Delahunt

Moth Olfactory System

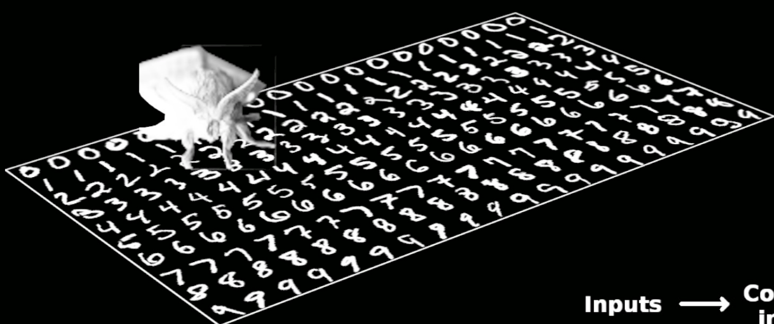


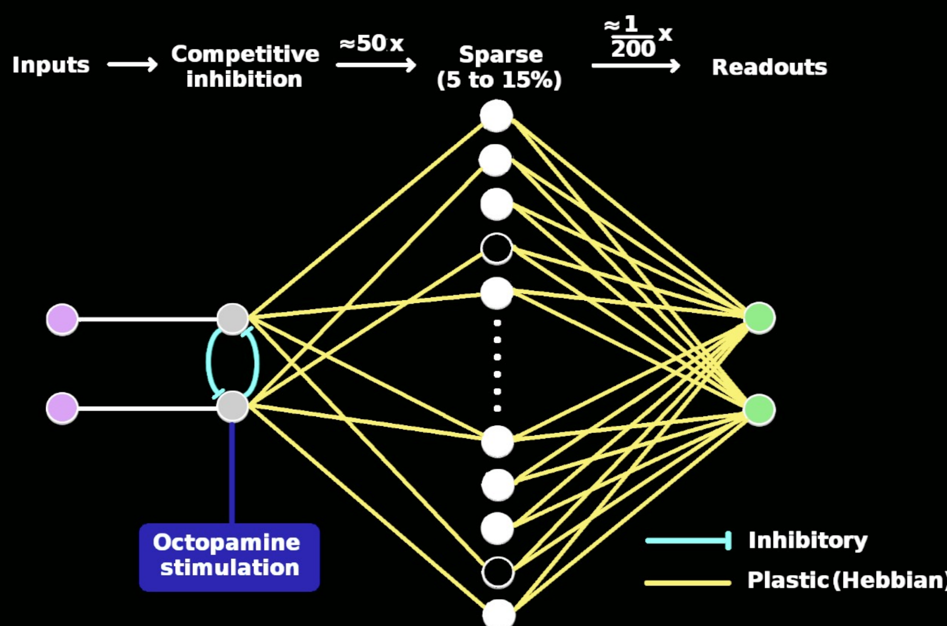
Riffell et al. Science 2013
Campbell et al. J Neuro 2013
Olson et al. Neuron 2010
Turner et al. J NeuroPhysiol 2008 Hong, Wilson. Neuron 2015

Gupta, Stopfer. J NeuroSci 2012
Silbering et al. J NeuroSci 2003
Galizia. Eur J NeuroSci 2014
Caron et al. Nature 2013

Delahunt, Riffell, Kutz (2018) FNS

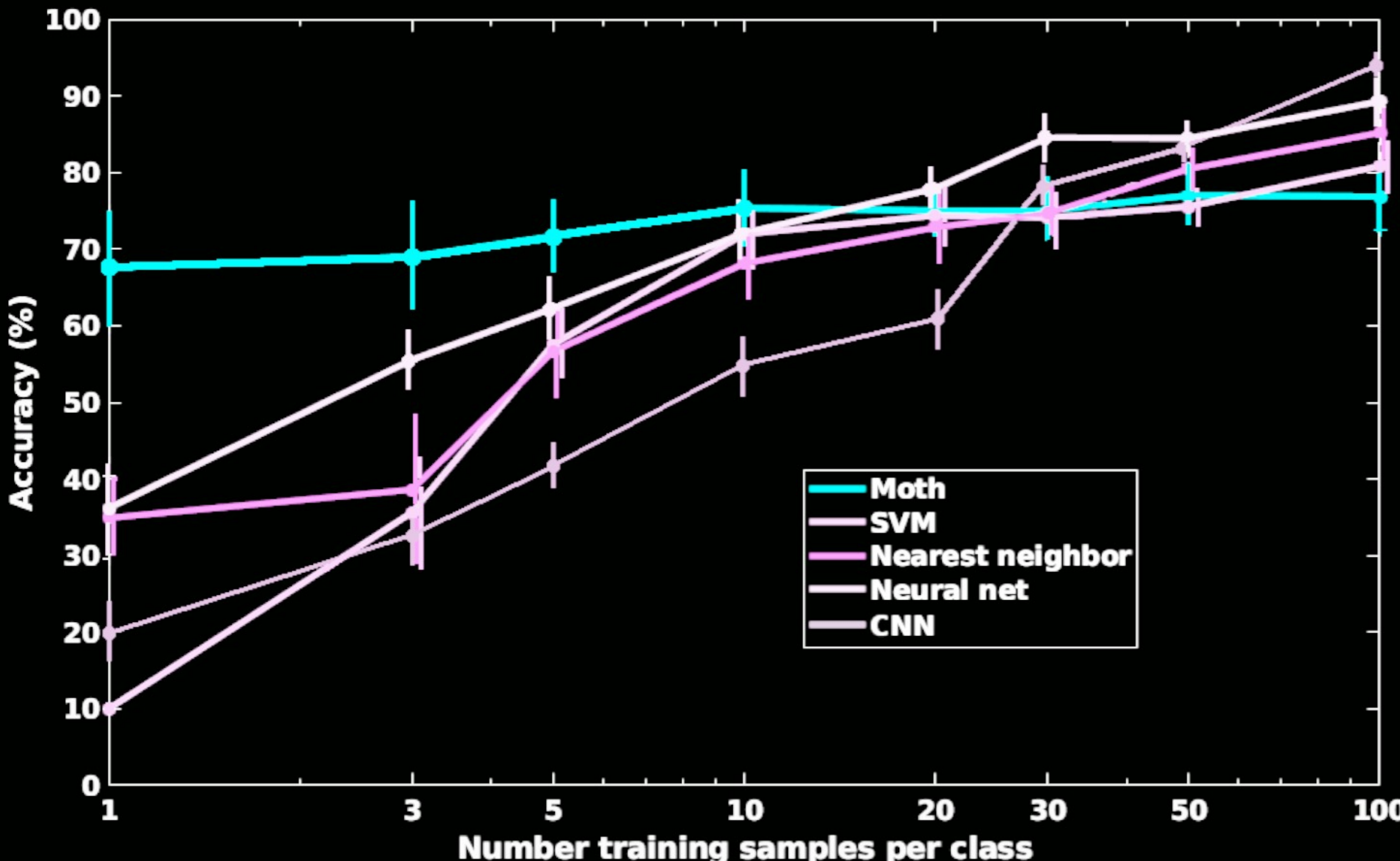
Rapid Learning in NNs





Delahunt & Kutz (2018) arxiv

Comparisons



Conclusion

Model Discovery: Sparse regression provides parsimonious dynamical models

Coordinates: Learning Koopman embeddings can provide optimal basis for dynamics

Neural Networks: Structure and function matter

- Connect discovery and coordinates
- Structure can lead to fast (one-shot) learning with limited data
- Discovery of improved coordinate embeddings through decoding

COMING SOON: A multi scale physics challenge set

Coming Soon

Multiscale Physics Challenge Data Set: Taking on the model of computer vision

Coming Soon

Multiscale Physics Challenge Data Set: Taking on the model of computer vision