

DATA-DRIVEN DISCOVERY OF GOVERNING PHYSICAL LAWS AND COORDINATES FOR ENGINEERING AND PHYSICS

- Model discovery
- Manifolds & Embeddings
- Measurement & Sensors

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faculty.washingon.edu/kutz

See link to "open source lectures"



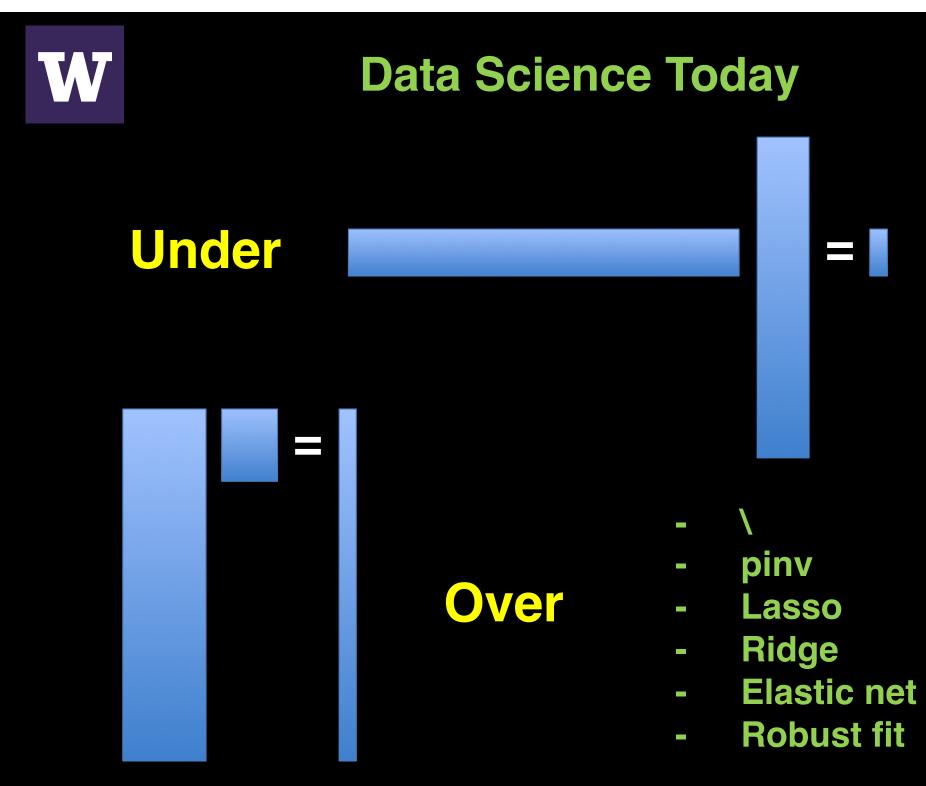
Part 0 Applied Optimization & Machine Learning



Part 0 Applied Optimization is Machine Learning



Ax=b







subject to

min g(x)

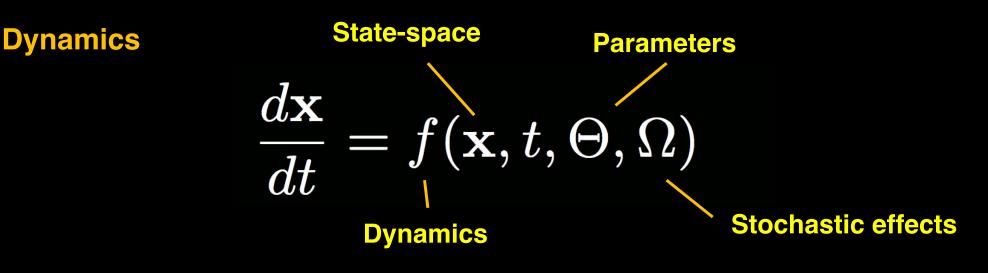


f(A,x)=b

subject to

min g(x)

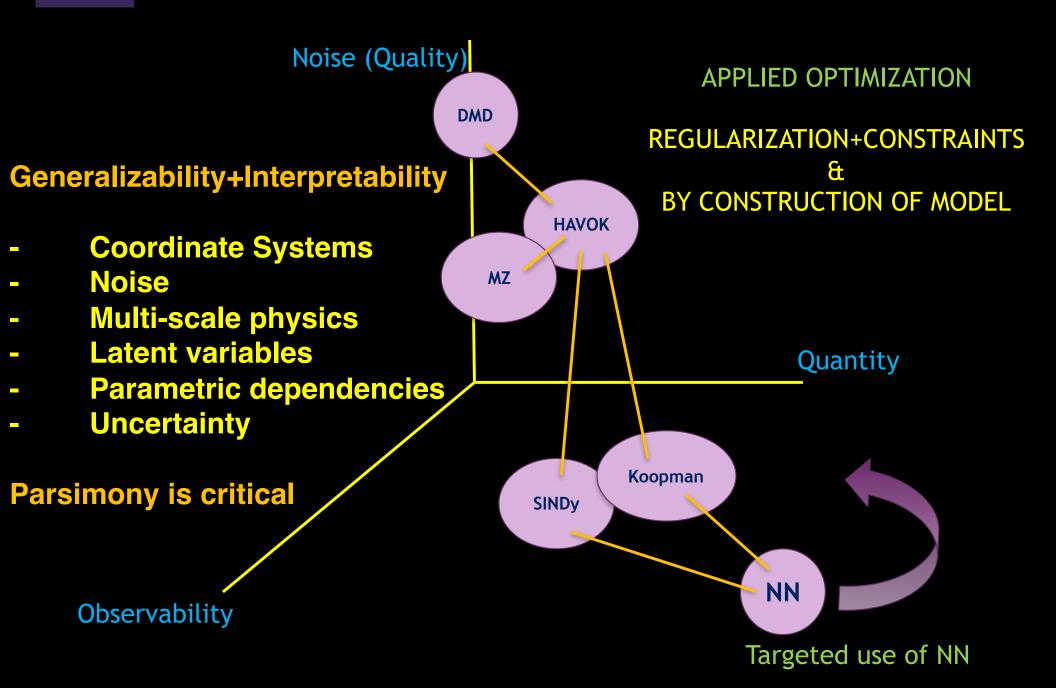




Measurement

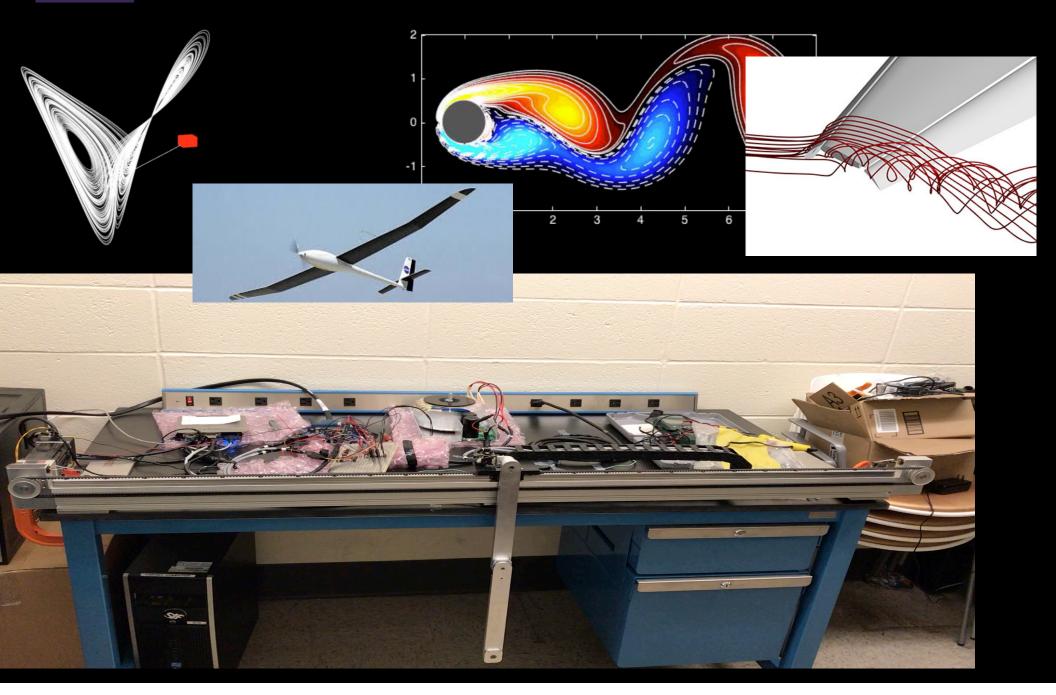
$$\mathbf{y}(t_k) = h(t_k, \mathbf{x}(t_k), \Xi)$$
Measurement model
Measurement noise

W A Diversity of Strategies





Diverse Models





Part 1 Model Discovery



Steven Brunton

Mechanical Engineering University of Washington



Joshua Proctor

Institute for Disease Modeling



Generic nonlinear , time-dependent, parametric system

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

Measurements (assimilation)

$$G(\mathbf{x}, t_k) = \mathbf{0}$$



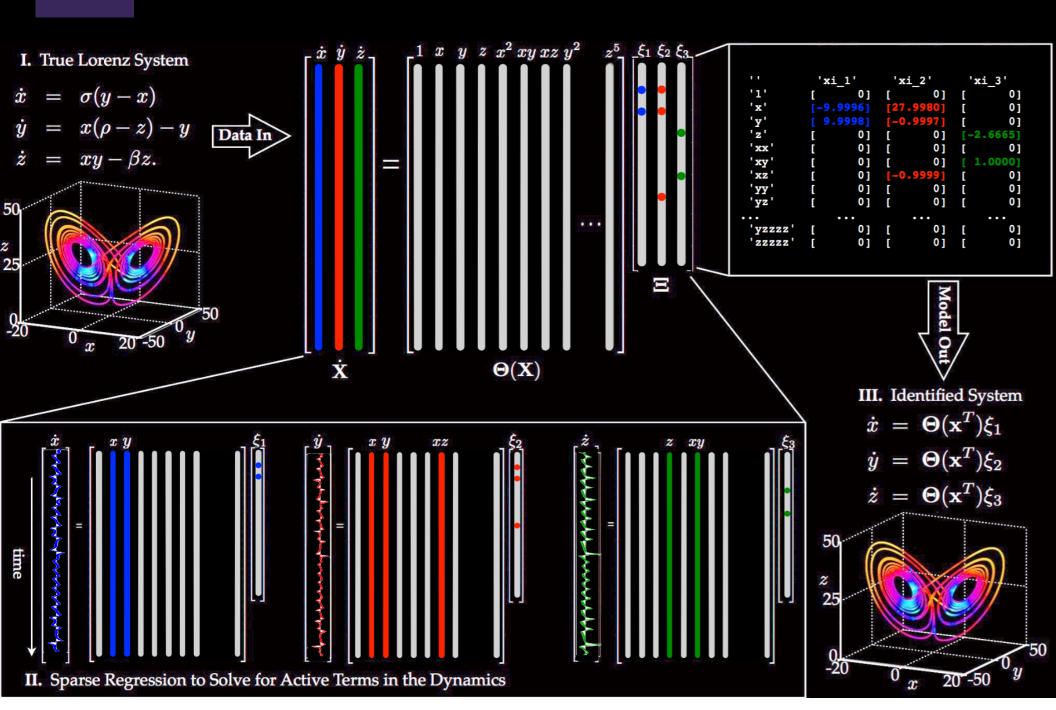
Limited by your imagination

$$\boldsymbol{\Theta}(\mathbf{X}) = \begin{bmatrix} \mathbf{I} & \mathbf{I} & \mathbf{I} & \mathbf{I} \\ \mathbf{1} & \mathbf{X} & \mathbf{X}^{P_2} & \mathbf{X}^{P_3} & \cdots & \sin(\mathbf{X}) & \cos(\mathbf{X}) & \sin(2\mathbf{X}) & \cos(2\mathbf{X}) & \cdots \\ \mathbf{I} & \mathbf{I} \end{bmatrix}$$

2nd degree polynomials

$$\mathbf{X}^{P_2} = \begin{bmatrix} x_1^2(t_1) & x_1(t_1)x_2(t_1) & \cdots & x_2^2(t_1) & x_2(t_1)x_3(t_1) & \cdots & x_n^2(t_1) \\ x_1^2(t_2) & x_1(t_2)x_2(t_2) & \cdots & x_2^2(t_2) & x_2(t_2)x_3(t_2) & \cdots & x_n^2(t_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ x_1^2(t_m) & x_1(t_m)x_2(t_m) & \cdots & x_2^2(t_m) & x_2(t_m)x_3(t_m) & \cdots & x_n^2(t_m) \end{bmatrix}$$

Sparse Identification of Nonlinear Dynamics (SINDy)





Nonlinear Systems ID

I. Collect Data

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^{T}(t_{1}) \\ \mathbf{x}^{T}(t_{2}) \\ \vdots \\ \mathbf{x}^{T}(t_{m}) \end{bmatrix} = \begin{bmatrix} x_{1}(t_{1}) & x_{2}(t_{1}) & \cdots & x_{n}(t_{1}) \\ x_{1}(t_{2}) & x_{2}(t_{2}) & \cdots & x_{n}(t_{2}) \\ \vdots & \vdots & \ddots & \vdots \\ x_{1}(t_{m}) & x_{2}(t_{m}) & \cdots & x_{n}(t_{m}) \end{bmatrix} \int \mathbf{x}^{T}(t_{1}) \\ \mathbf{x}^{T}(t_{2}) \\ \vdots \\ \mathbf{x}^{T}(t_{m}) \end{bmatrix} = \begin{bmatrix} \dot{x}_{1}(t_{1}) & \dot{x}_{2}(t_{1}) & \cdots & \dot{x}_{n}(t_{1}) \\ \dot{x}_{1}(t_{2}) & \dot{x}_{2}(t_{2}) & \cdots & \dot{x}_{n}(t_{2}) \\ \vdots & \vdots & \ddots & \vdots \\ \dot{x}_{1}(t_{m}) & \dot{x}_{2}(t_{m}) & \cdots & \dot{x}_{n}(t_{m}) \end{bmatrix} .$$

2. Build Library of Candidate Nonlinearities

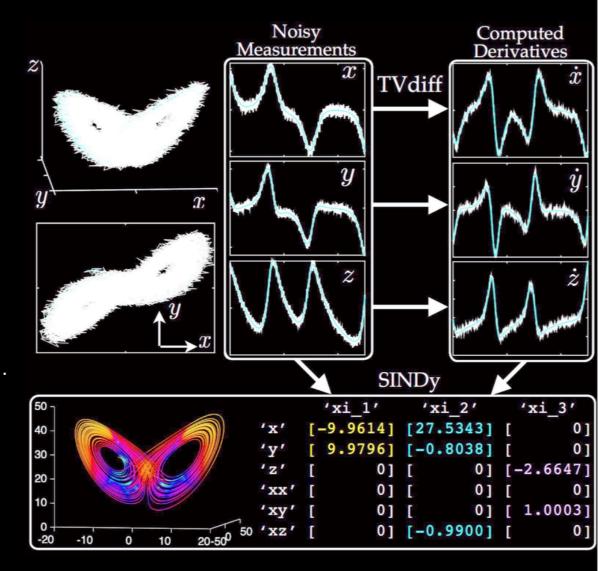
$$\Theta(\mathbf{X}) = \left[\begin{array}{cccccccc} | & | & | & | \\ \mathbf{1} & \mathbf{X} & \mathbf{X}^{P_2} & \mathbf{X}^{P_3} & \cdots & \sin(\mathbf{X}) & \cos(\mathbf{X}) & \cdots \\ | & | & | & | & | & | & | & | & | \end{array}\right]$$

3. Sparse Regression to Find Active Terms

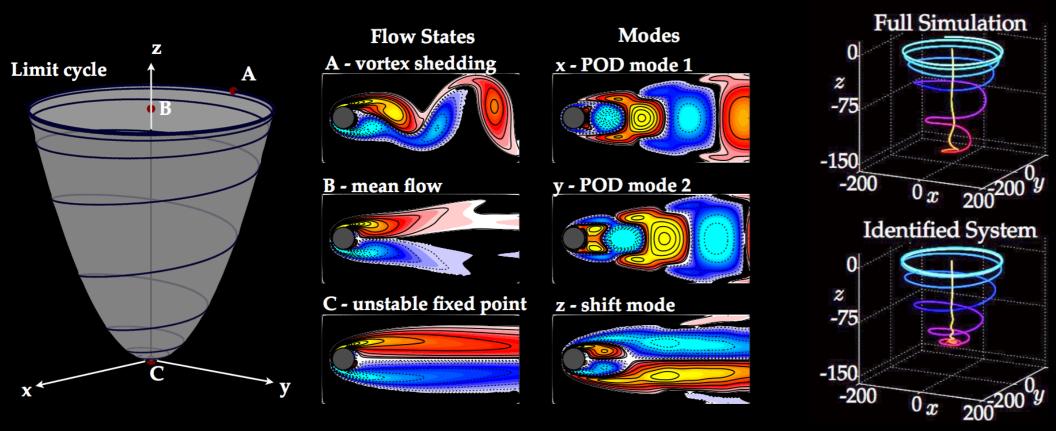
 $\dot{\mathbf{X}} = \mathbf{\Theta}(\mathbf{X}) \mathbf{\Xi}.$

4. Nonlinear Model

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) = \mathbf{\Xi}^T (\mathbf{\Theta}(\mathbf{x}^T))^T$$



Identifying Slow Manifolds



30 years of progress

W

$$\dot{x} = \mu x - \omega y + Axz$$

 $\dot{y} = \omega x + \mu y + Ayz$
 $\dot{z} = -\lambda(z - x^2 - y^2).$

I. Hopf bifurcations as path to turbulence Ruelle & Takens, Communications in Mathematical Physics, 1971

2. Vortex shedding and Hopf bifurcation Jackson, Journal of Fluid Mechanics, 1987.

3. Mean-field model with slow manifold Noack, Afanasiev, Morzynski, Tadmor, & Thiele, Journal of Fluid Mechanics, 2003.

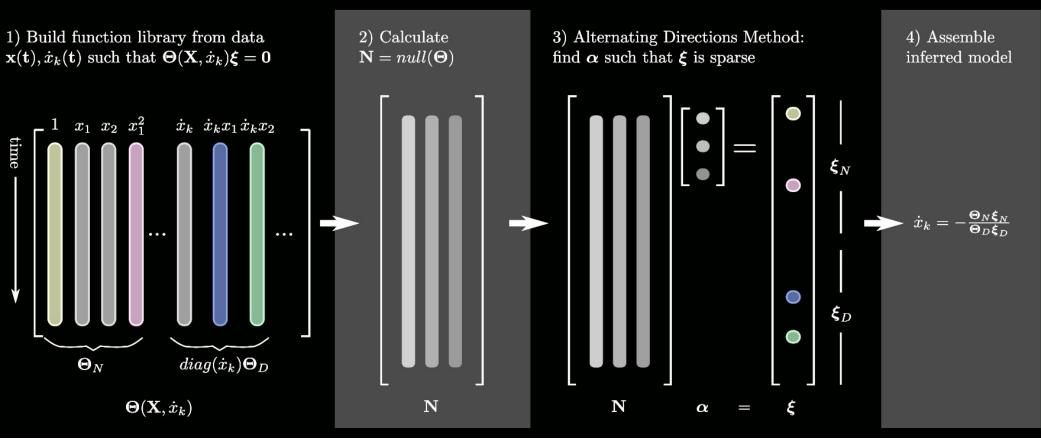


Modifications: Implicity-SINDy



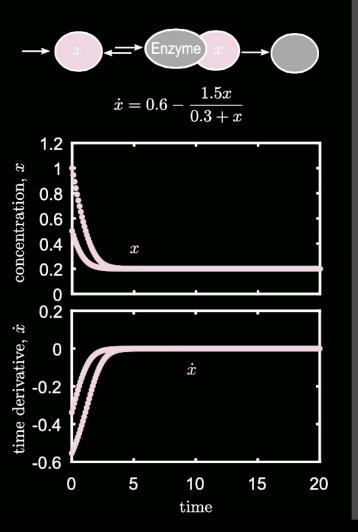
Niall Mangan

 $= \frac{f_N(\mathbf{x})}{f_D(\mathbf{x})}$ \dot{x}_k =

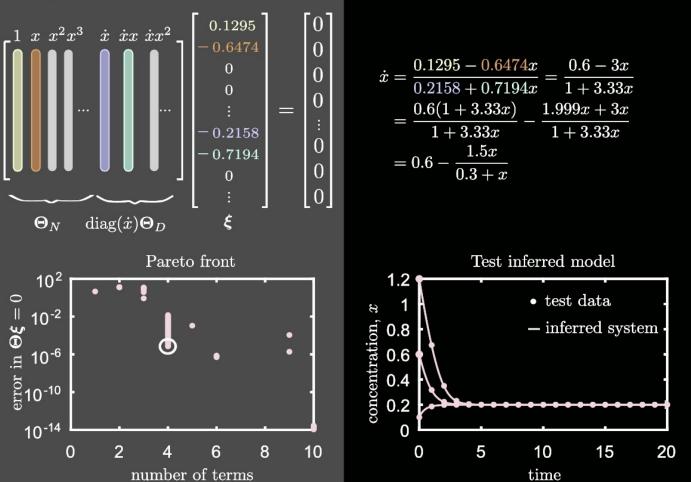


W Michaelis-Menten: enzymatic reaction

1) Generate test data from system:



2) Build functional library. Sparsely select terms and find λ where error drops on Pareto front:

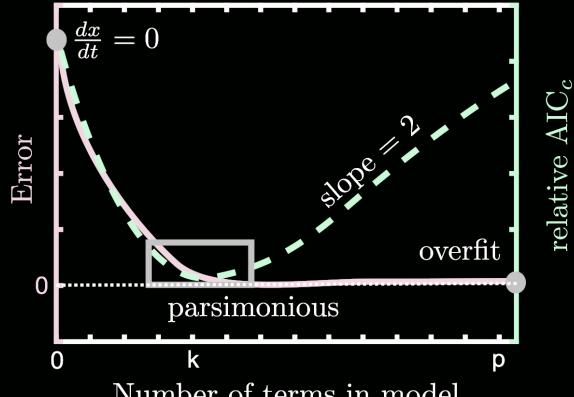


3) Construct inferred model and

conditions:

compare with data from new initial

Parsimony



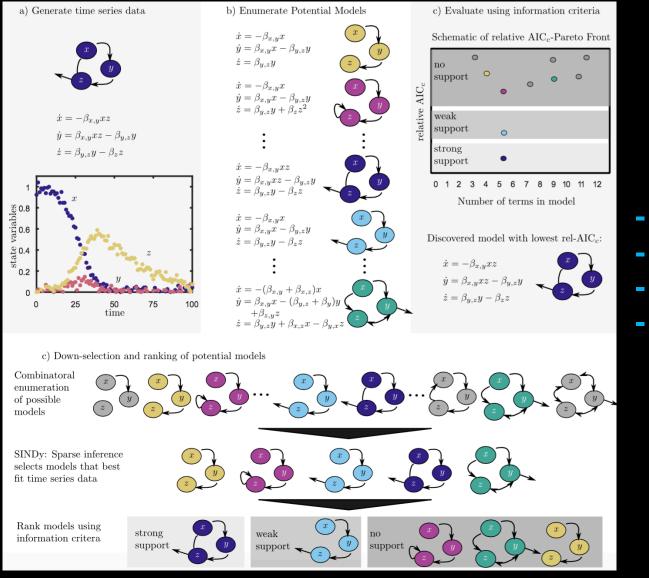
W

Number of terms in model

$$AIC_j = 2k - 2\ln(L(\mathbf{x}, \hat{\mu}))$$

 $L(\mathbf{x}, \mu) = P(\mathbf{x}|\mu)$ is the likelihood function

Model Selection and Information Theory

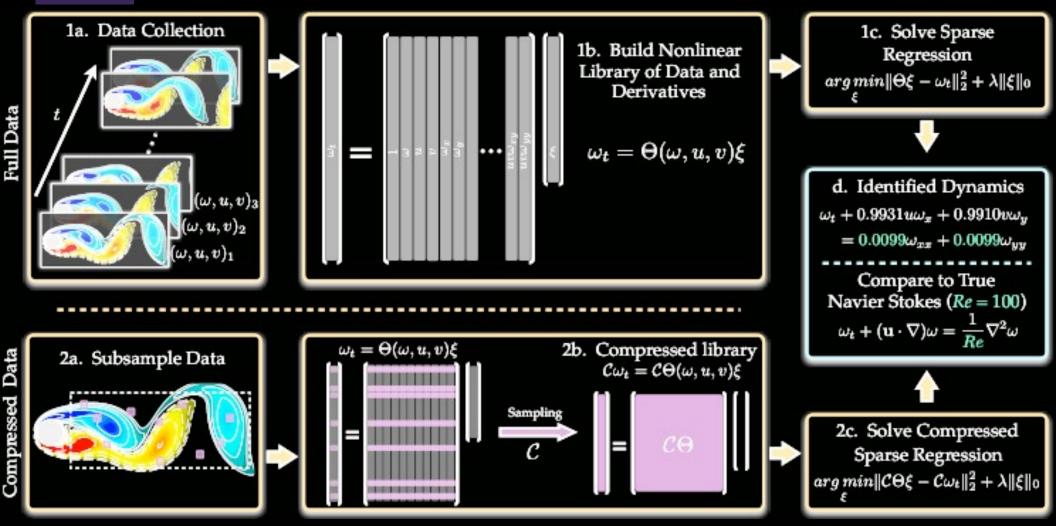


Model Selection

- 1950s KL divergence
- Early 70s AIC (Akaike)
- 78 BIC (G. Schwarz)
- BIC/AIC limited # of models



Discovering PDEs

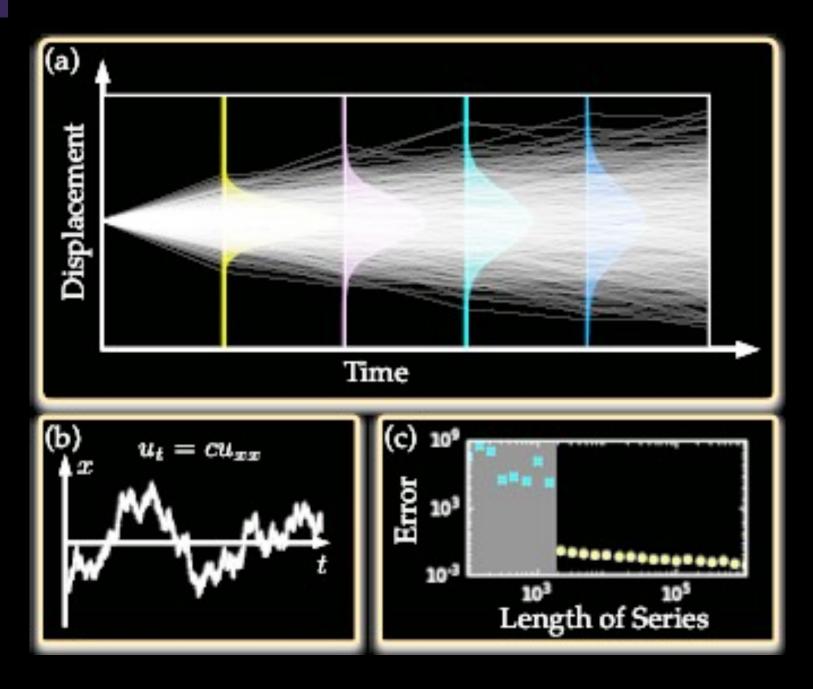




Sam Rudy

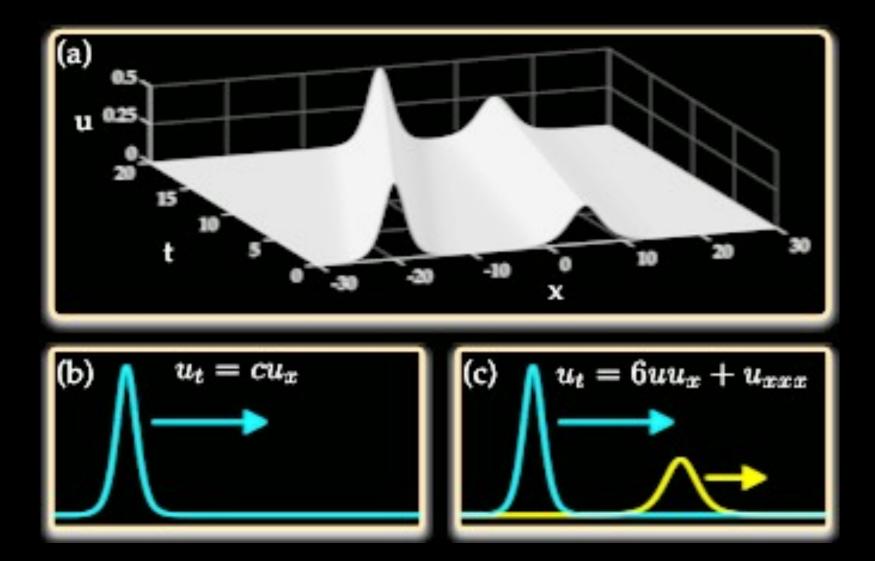


Lagrangian Measurements





Disambiguation

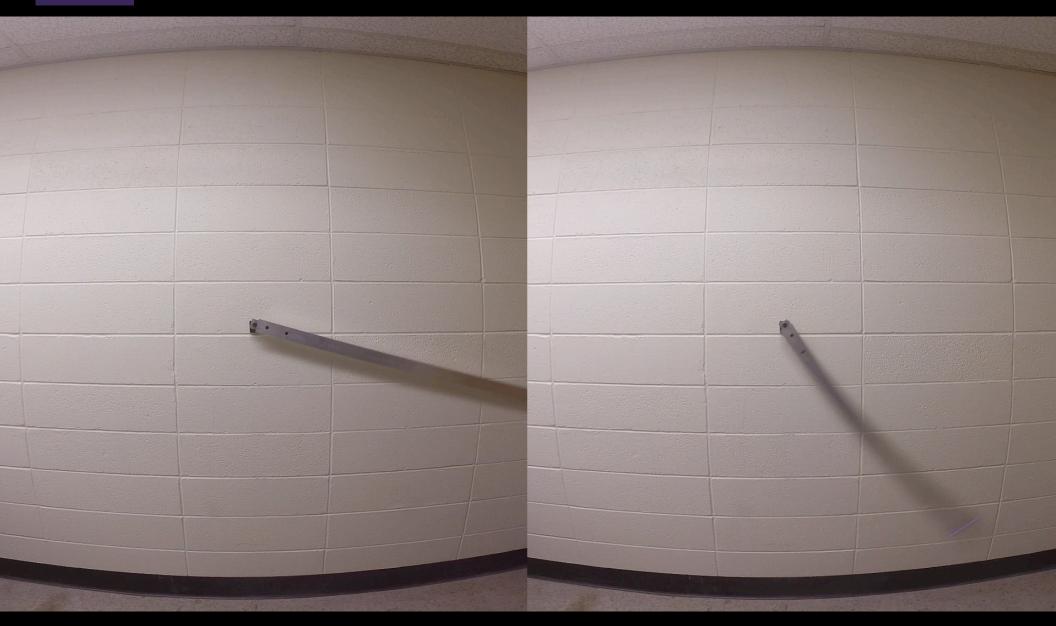




PDE		Form	Error (no noise, noise)	Discretization
KdV	,	$u_t + 6uu_x + u_{xxx} = 0$	$1\% \pm 0.2\%, 7\% \pm 5\%$	$x \in [-30, 30], n = 512, t \in [0, 20], m = 201$
Burg	gers	$u_t + u u_x - \epsilon u_{xx} = 0$	$0.15\%{\pm}0.06\%, 0.8\%{\pm}0.6\%$	$x \in [-8, 8], n = 256, t \in [0, 10], m = 101$
Schro	odinger	$iu_t+rac{1}{2}u_{xx}-rac{x^2}{2}u=0$	$0.25\%{\pm}0.01\%, 10\%{\pm}7\%$	$x \in [-7.5, 7.5], n = 512, t \in [0, 10], m = 401$
		$iu_t+rac{1}{2}u_{xx}+ u ^2u=0$	$0.05\%{\pm}0.01\%,3\%{\pm}1\%$	$x \in [-5, 5], n = 512, t \in [0, \pi], m = 501$
KS		$u_t + uu_x + u_{xx} + u_{xxxx} = 0$	$1.3\%{\pm}1.3\%,70\%{\pm}27\%$	$x \in [0, 100], n = 1024, t \in [0, 100], m = 251$
R-D		$egin{aligned} &u_t=0.1 abla^2u+\lambda(A)u-\omega(A)v\ &v_t=0.1 abla^2v+\omega(A)u+\lambda(A)v\ &A=u^2+v^2, \omega=-eta A^2, \lambda=\!1\!-\!A^2 \end{aligned}$	$0.02\% \pm 0.01\%, 3.8\% \pm 2.4\%$	$x, y \in [-10, 10], n=256, t \in [0, 10], m=201$ subsample $3 \cdot 10^5$
Navier	Stokes	$\omega_t + (\mathbf{u} \cdot abla) \omega = rac{1}{Re} abla^2 \omega$	$1\%\pm0.2\%$, $7\%\pm6\%$	$\substack{x \in [0, 9], n_x = 449, y \in [0, 4], n_y = 199, \ t \in [0, 30], m = 151, \text{ subsample } 3 \cdot 10^5}$



Experiments



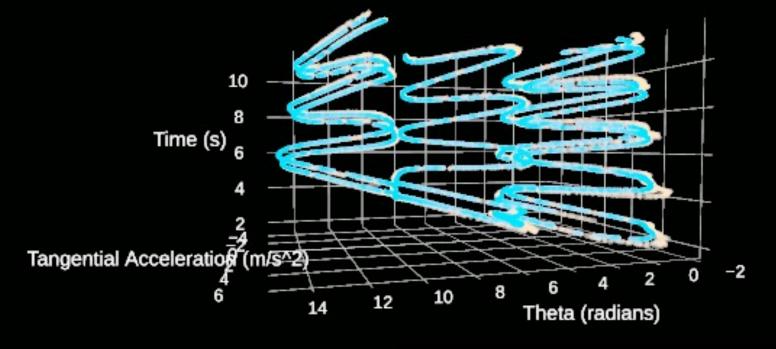


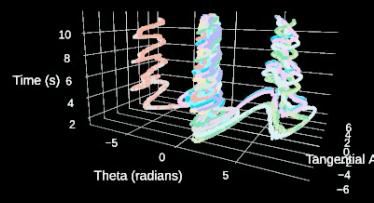
Arduino Magic

Data vs. SINDy Plot



(77854, 2) (77854, 2)
With -1 jobs, fit and predict STRidge took 5.747981 seconds.
dx_0 / dt = 1.0*x_1
dx_1 / dt = -0.1460697460858498*x_1+-3.9120253716489075*sin(x_0)







KEY CHALLENGES

- Limited measurements & data
- Noise
- Multi-scale physics
- Latent variables
- Parametric dependencies
- Stochastic systems

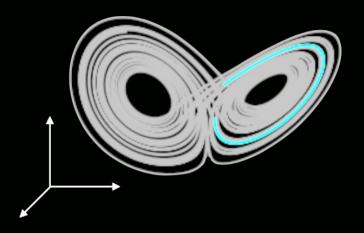


Multiscale Systems

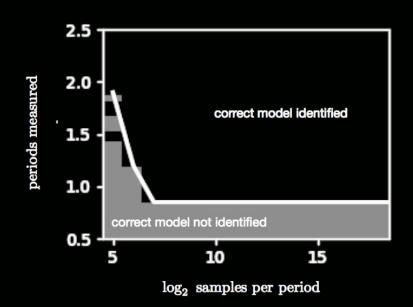


Limits of Model Discovery

Lorenz system

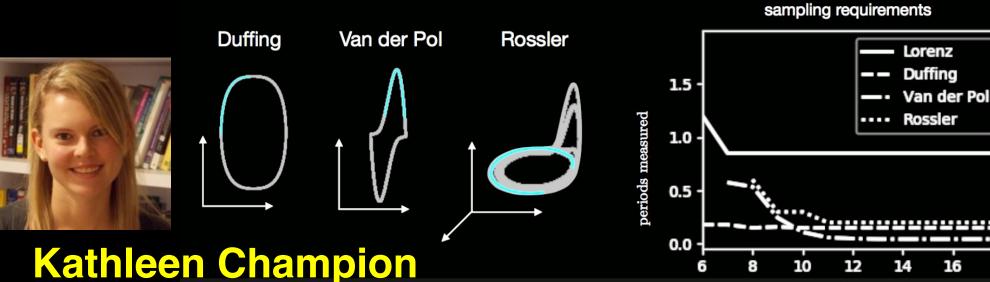


SINDy sampling requirements



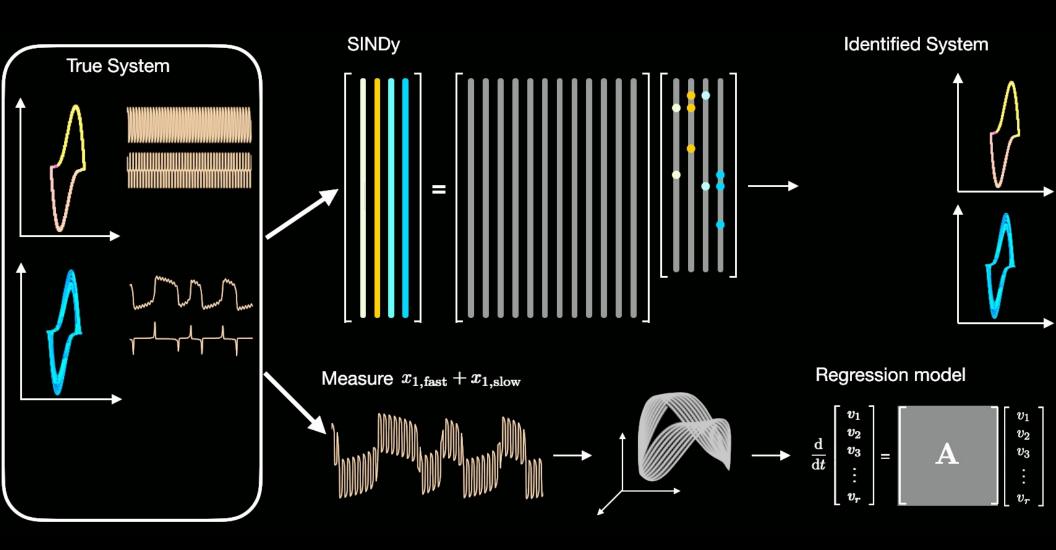
log₂ samples per period

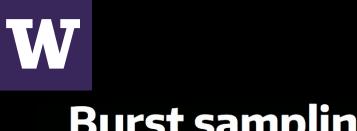
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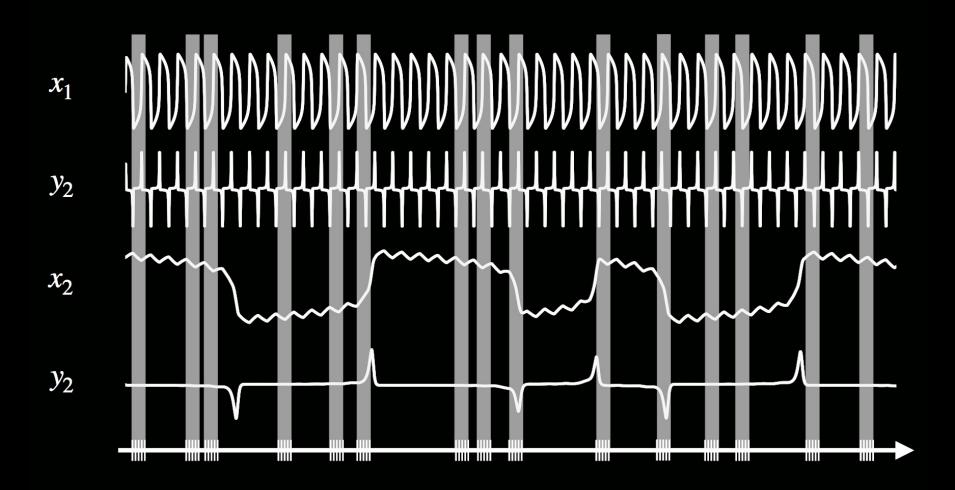
Multiscale Physics Discovery

W





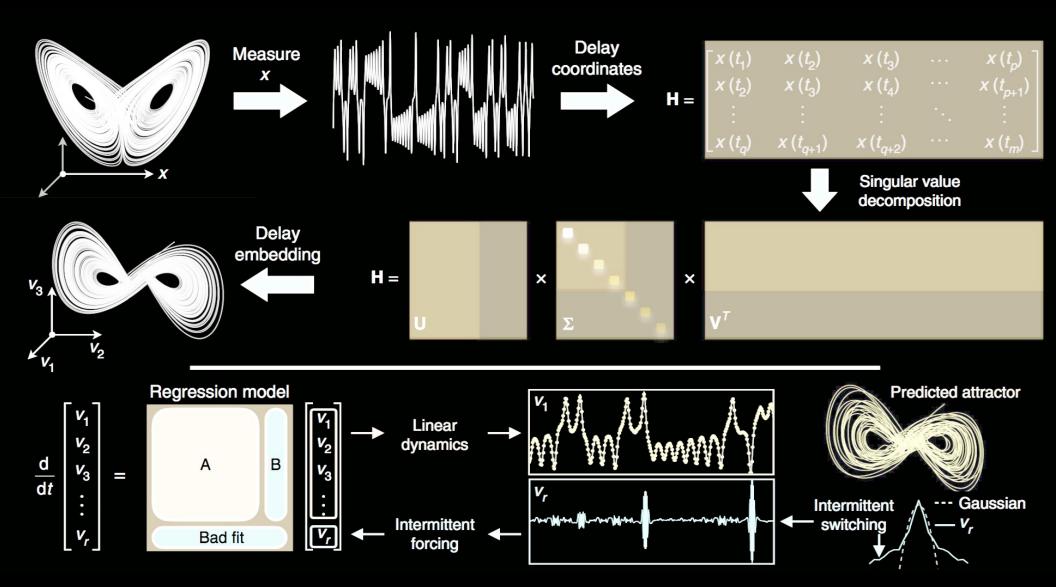
Burst sampling





Latent Variables



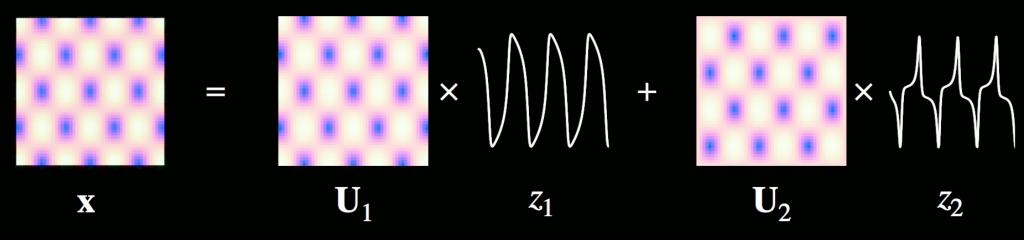




Latent variables

 $\mathbf{x} = \mathbf{U}_1 z_1 + \mathbf{U}_2 z_2$

 $\dot{z}_1 = z_2$ $\dot{z}_2 = \mu(1 - z_1^2)z_2 - z_1$



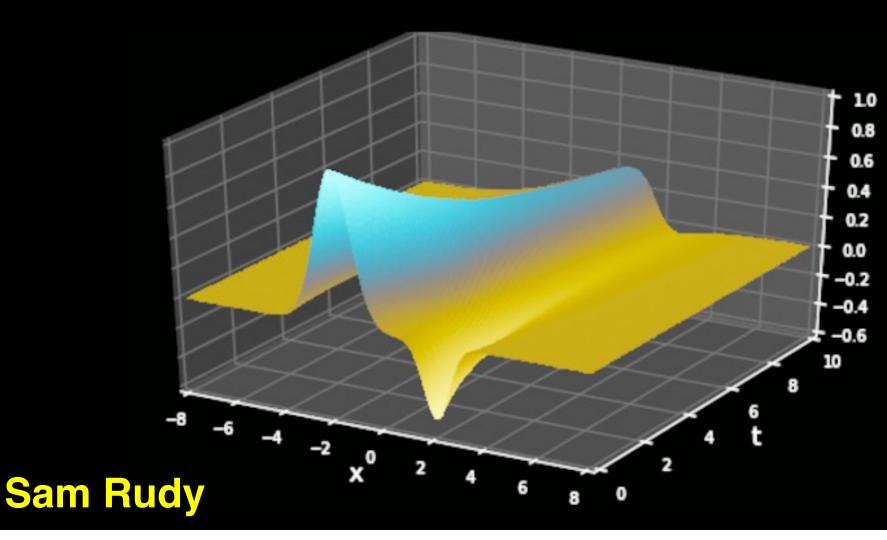


Parametric Systems



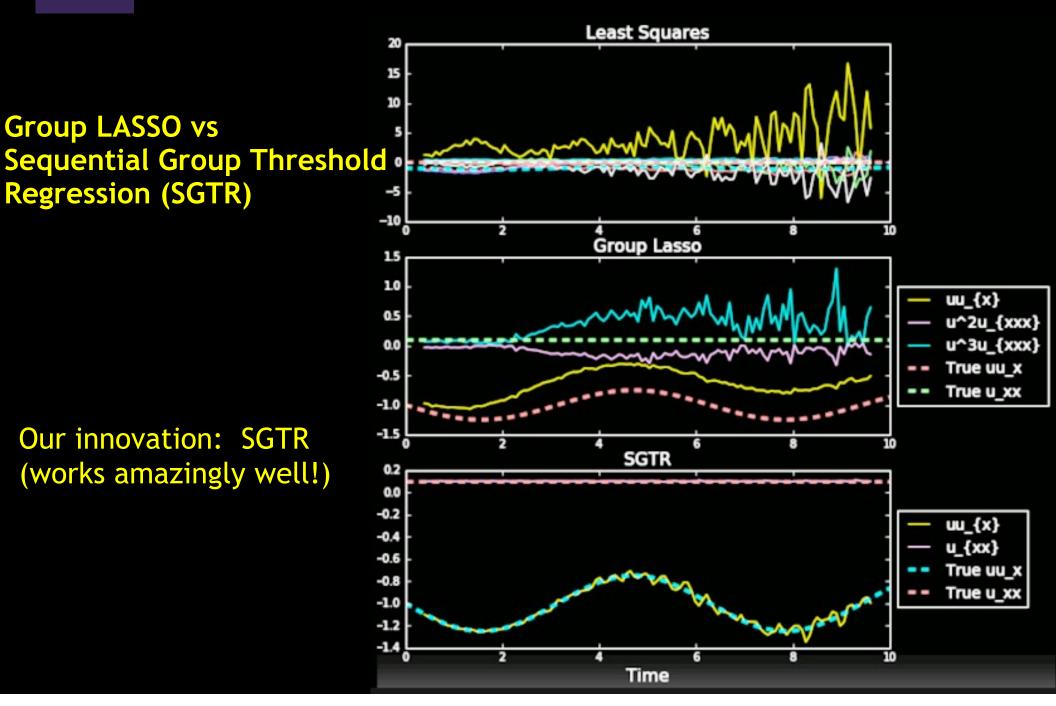
Parametric Burgers

$$u_t + \left(1 + \frac{1}{4}\sin(t)\right)uu_x - Du_{xx} = 0$$

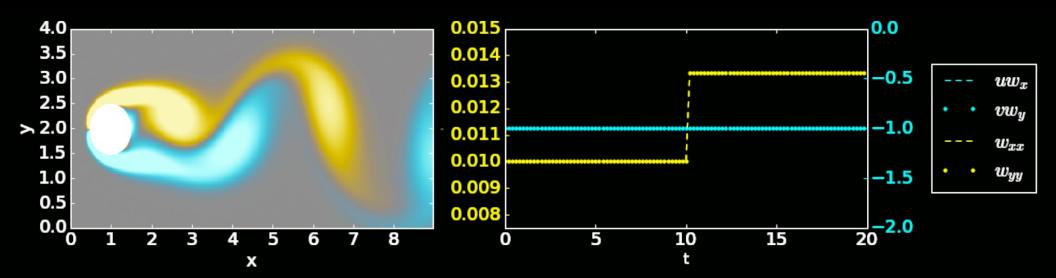


Parametric Discovery

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Parametric Dependence



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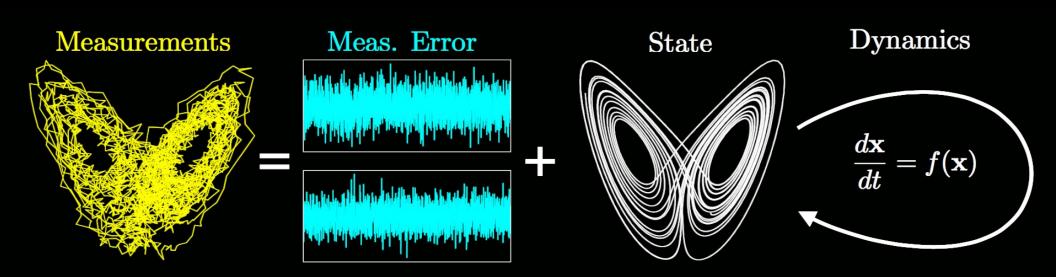
$$u_{t} = (c(x)u)_{x} + \epsilon u_{xx}$$

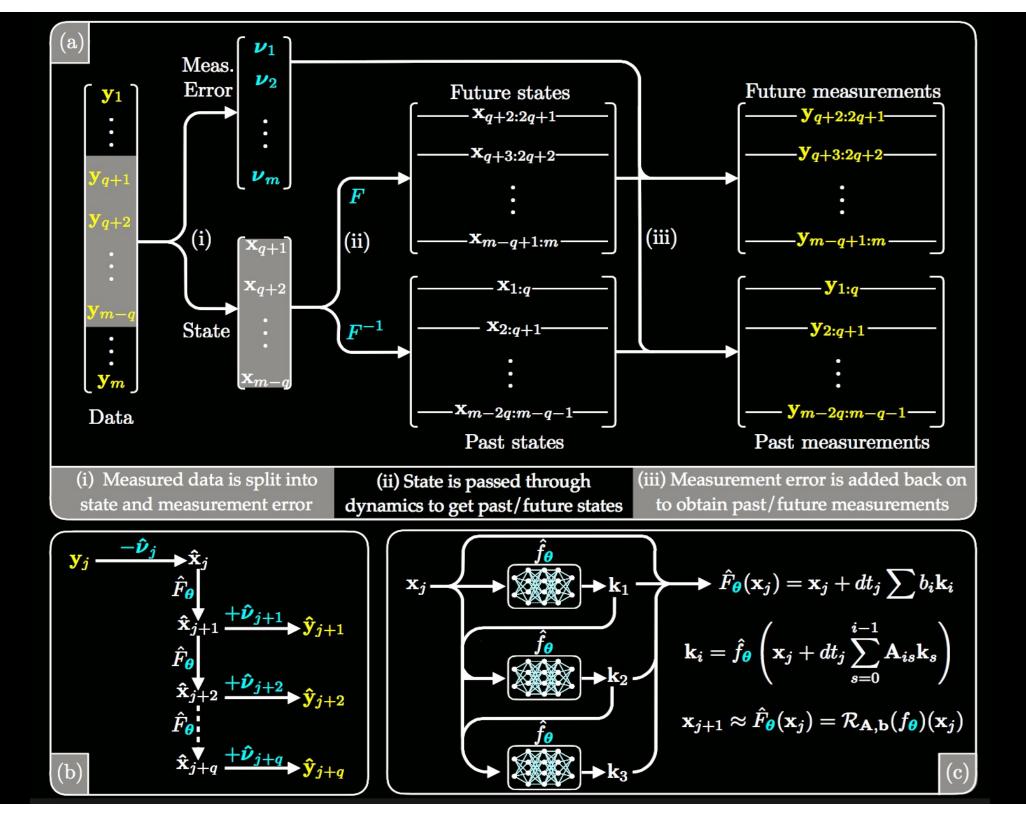
$$\int_{a}^{b} \frac{1.5}{1.0} \int_{a}^{1.5} \frac{1.5}{0.0} \int_{a}^{0.5} \frac{1.5}{0.$$

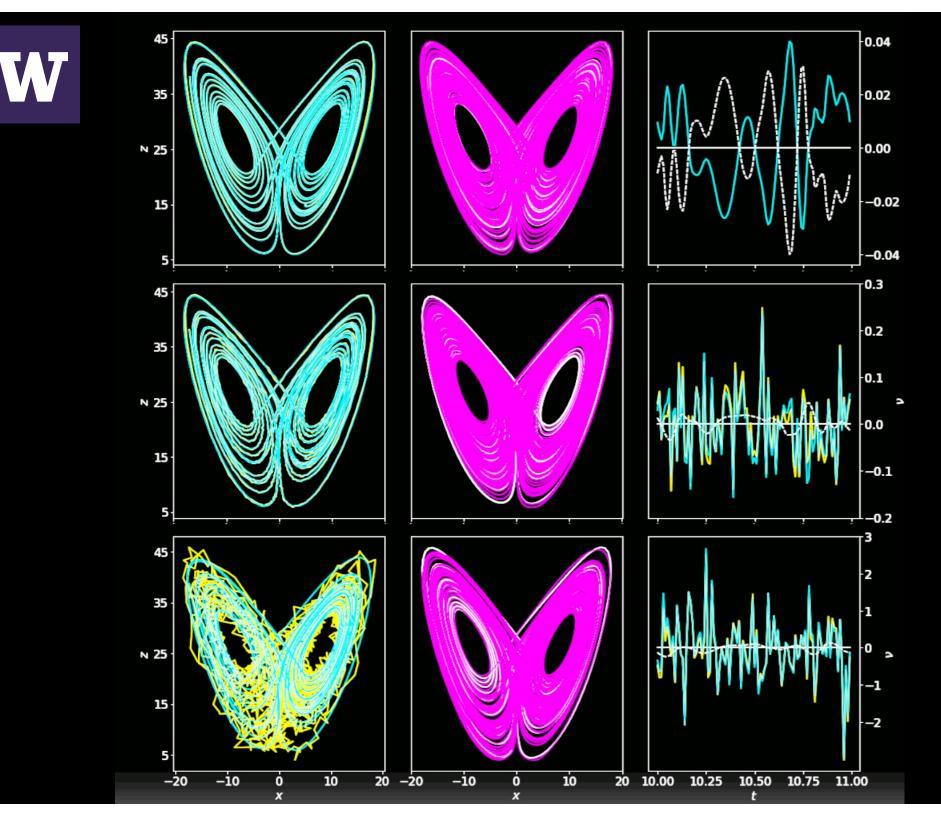


Noise





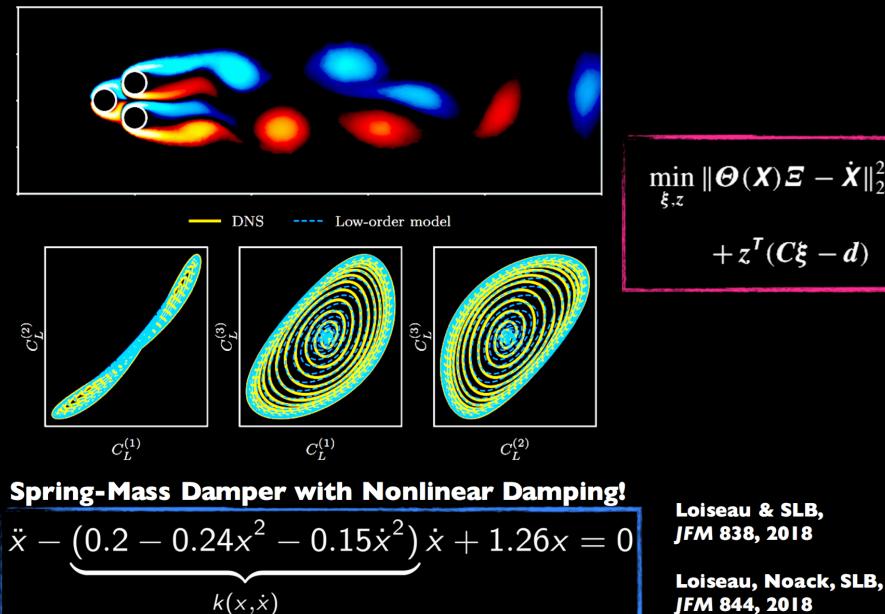






Control

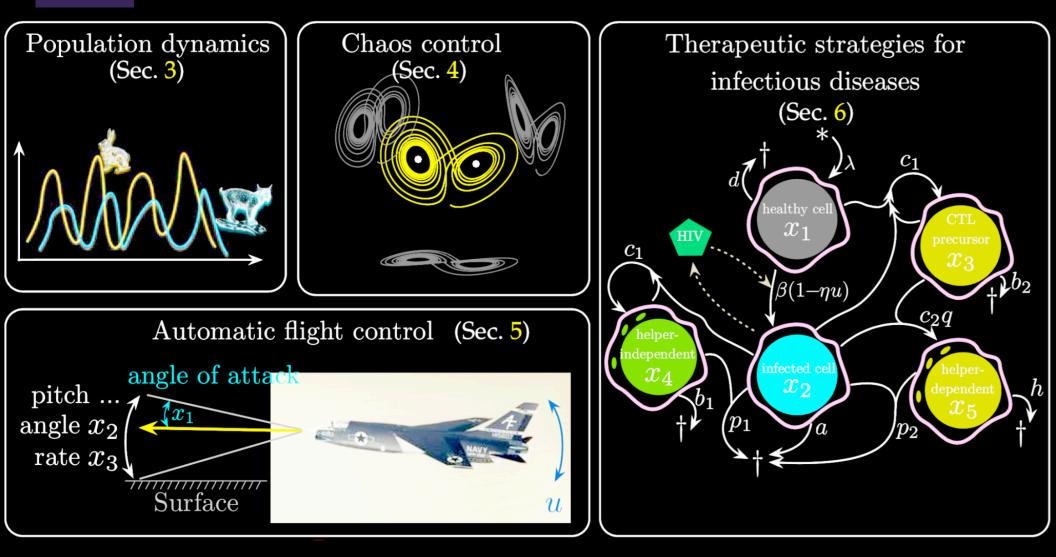
W Adding Energy Constraints



 $\min \|\boldsymbol{\Theta}(\boldsymbol{X})\boldsymbol{\Xi} - \dot{\boldsymbol{X}}\|_2^2$ $+z^{T}(C\xi-d)$

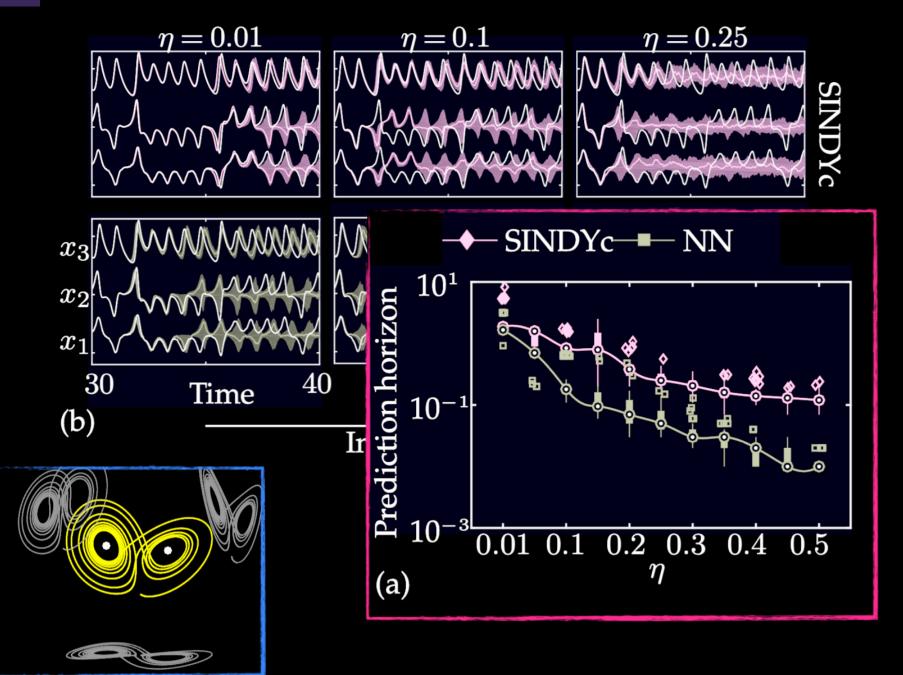
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SINDY + MPC





SINDY + MPC





SINDy Innovations

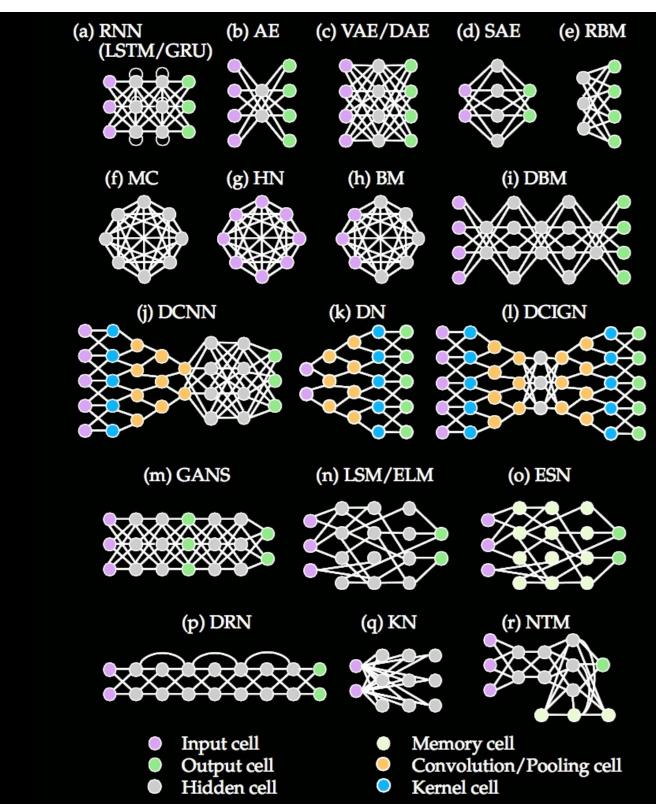
Schaeffer -- corrupt data, PDEs, integral formulation, convergence Dongbin Shu & co-workers (2018) – Sampling strategies Guang Lin & co-workers (2018) -- Uncertainty Metrics

Zheng, Askham, Brunton, Kutz & Aravkin (2018) – SR3 sparse relaxed regularized regression (for SINDy, LASSO, CS, TV, Matrix Completion ...)



Neural Nets





NN Zoo

W Neural Nets and Dynamics

% Simulate Lorenz system
dt=0.01; T=8; t=0:dt:T;
b=8/3; sig=10; r=28;

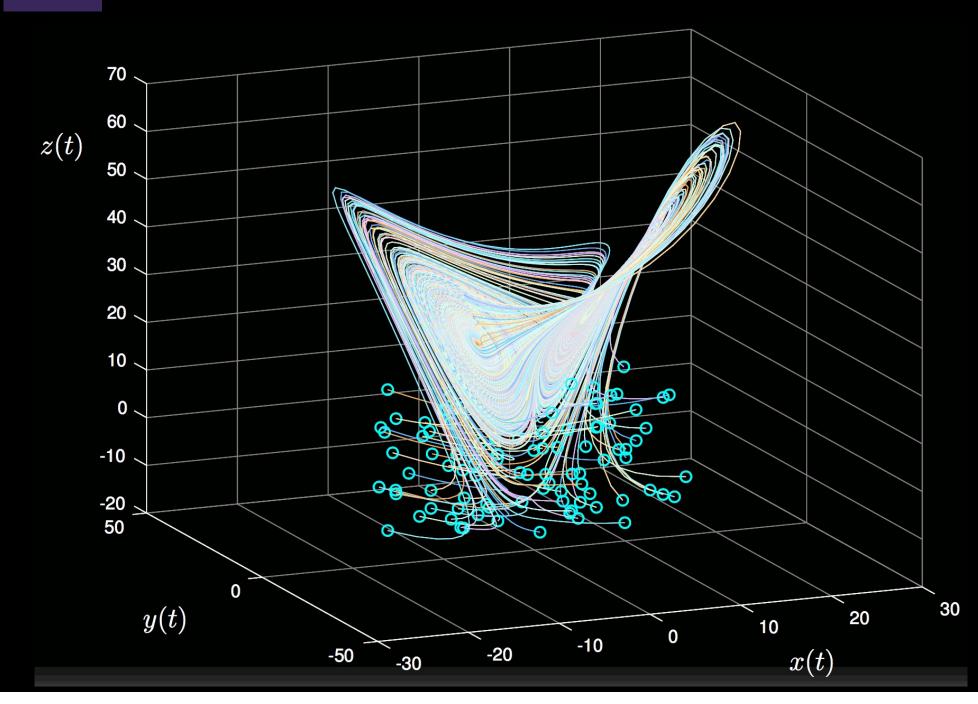
Lorenz = @(t,x)([sig * (x(2) - x(1)) ; ... r * x(1)-x(1) * x(3) - x(2) ; ... x(1) * x(2) - b*x(3)]); ode_options = odeset('RelTol', 1e-10, 'AbsTol', 1e-11);

input=[]; output=[]; for j=1:100 % training trajectories x0=30*(rand(3,1)-0.5); [t,y] = ode45(Lorenz,t,x0); input=[input; y(1:end-1,:)]; output=[output; y(2:end,:)]; plot3(y(:,1),y(:,2),y(:,3)), hold on plot3(x0(1),x0(2),x0(3),'ro')

end

Trajectories for Training

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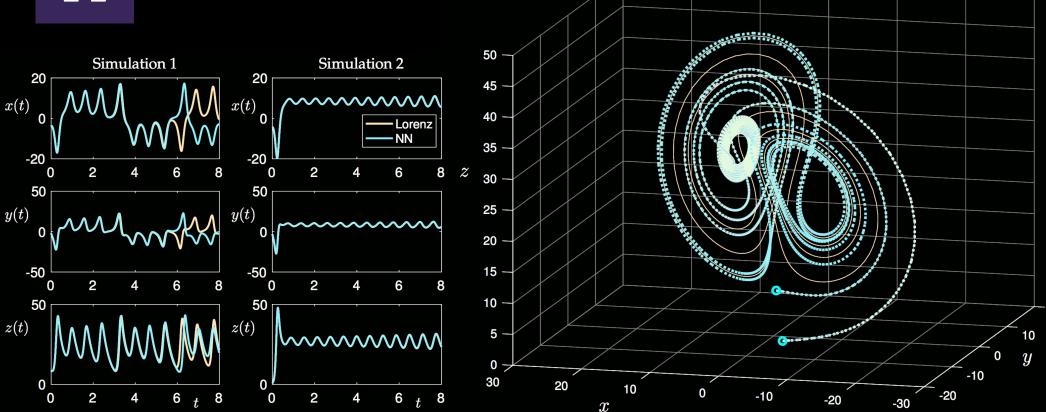




MATLAB NN



net = feedforwardnet([10 10 10]); net.layers{1}.transferFcn = 'logsig'; net.layers{2}.transferFcn = 'radbas'; net.layers{3}.transferFcn = 'purelin'; net = train(net, input.', output.'); W



ynn(1,:)=x0;
for jj=2:length(t)
 y0=net(x0);
 ynn(jj,:)=y0.'; x0=y0;
end
plot3(ynn(:,1),ynn(:,2),ynn(:,3),':','Linewidth',[2])



Part 2 Manifolds and Embeddings

Observables & Coordinates



Bernard Koopman 1931

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

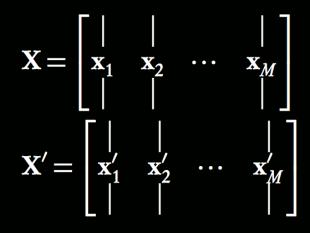
$$\frac{d\mathbf{x}}{dt} = \mathbf{N}(\mathbf{x}),$$

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 $\mathbf{g} : \mathcal{M} \to \mathbb{C}$ so that

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

Dynamic Mode Decomposition

Definition: Dynamic Mode Decomposition (Tu et al. 2014): *Suppose we have a dynamical system (1.17) and two sets of data*



with \mathbf{x}_k an initial condition to (1.17) and \mathbf{x}'_k it corresponding output after some prescribed evolution time τ with there being m initial conditions considered. The DMD modes are eigenvectors of

$$A_X = X'X^{\dagger}$$



W

where *†* denotes the Moore-Penrose pseudoinverse.

Travis Askham, optimized DMD

W Approximate Dynamical Systems

Linear dynamics (equation-free)

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

Eigenfunction expansion

K $\mathbf{\tilde{x}}(t) = \sum b_k \psi_k \exp(\omega_k t)$ k=1

Least-square fit

 $\|\mathbf{x}(t) - \mathbf{\tilde{x}}(t)\| \ll 1$



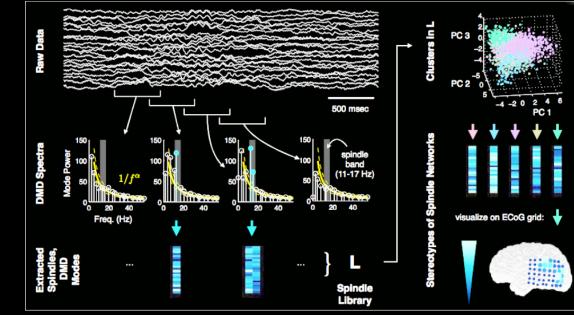
Some Applications

Dynamic Mode Decomposition for Financial Trading Strategies

Jordan Mann* and J. Nathan $Kutz^{\ddagger\dagger}$



ECOG recordings



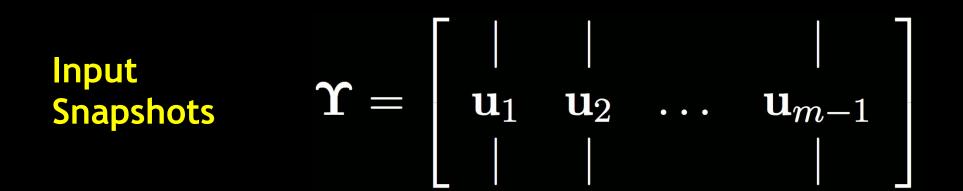
Erichson, Brunton & Kutz (2017) Brunton, Johnson, Ojemann & Kutz (2017)



DMD with Control

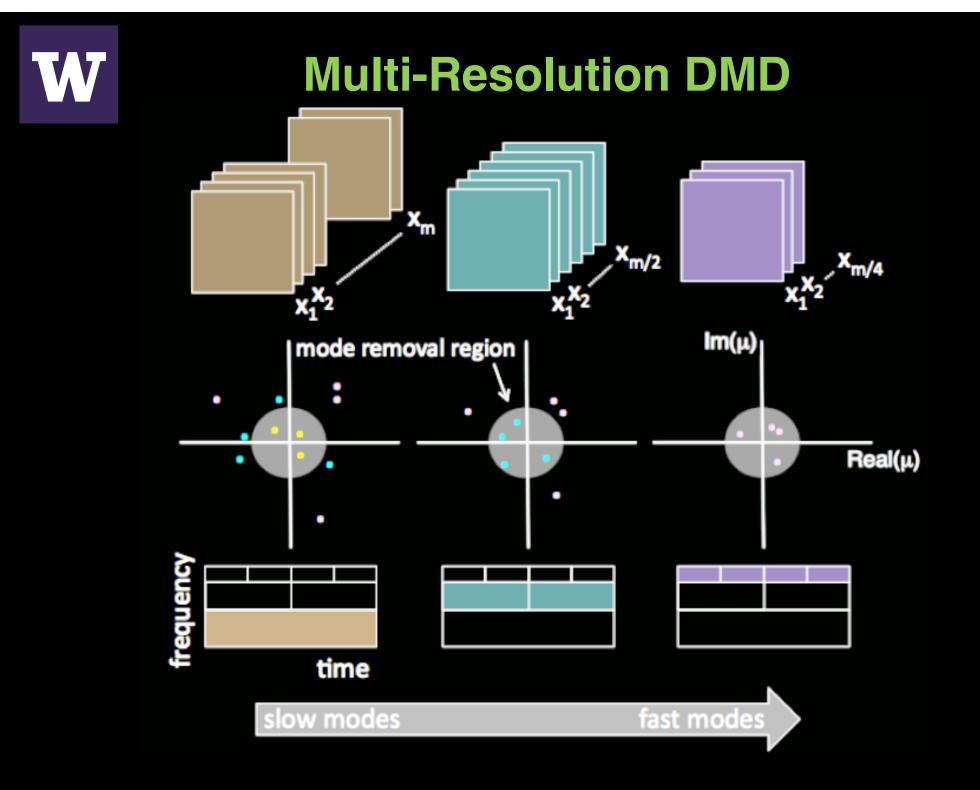
Input

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

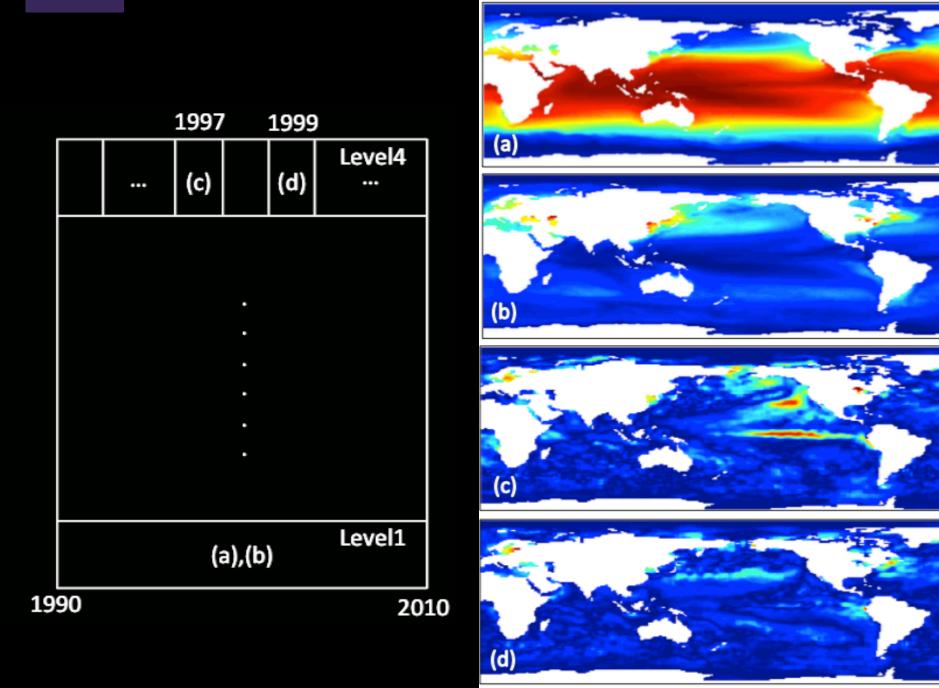


DMD generalization

$\mathbf{X}' \approx \mathbf{A}\mathbf{X} + \mathbf{B}\mathbf{\Upsilon}$



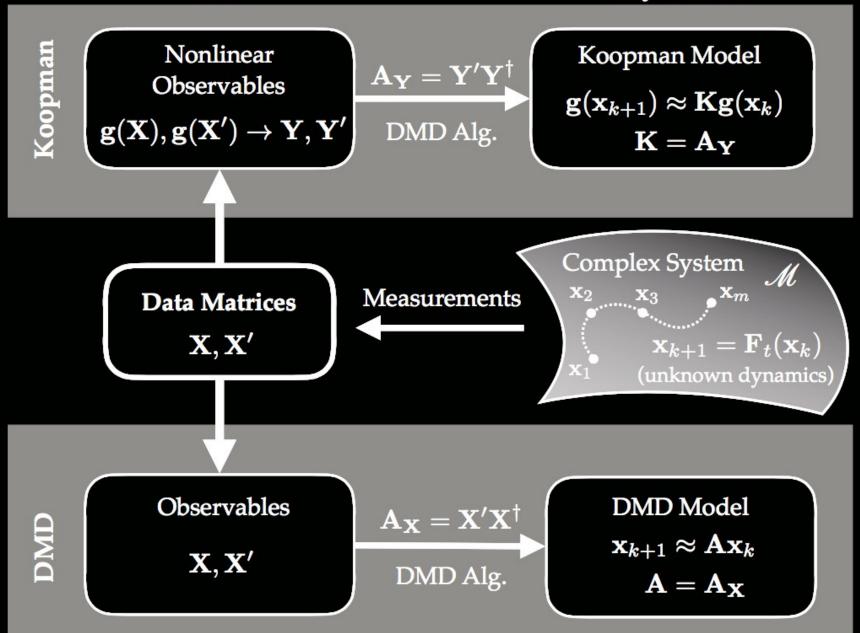
W SST data & El Nino (1990s-2010+)



WKoopman vs DMD: All about Observables!

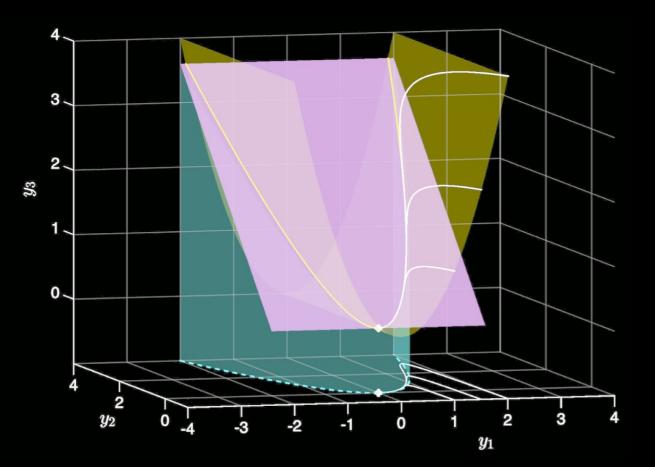
Data

Dynamics



Koopman Invariant Subspaces

$$\dot{x}_{1} = \mu x_{1} \\ \dot{x}_{2} = \lambda (x_{2} - x_{1}^{2})$$
 \implies
$$\frac{d}{dt} \begin{bmatrix} y_{1} \\ y_{2} \\ y_{3} \end{bmatrix} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \lambda & -\lambda \\ 0 & 0 & 2\mu \end{bmatrix} \begin{bmatrix} y_{1} \\ y_{2} \\ y_{3} \end{bmatrix}$$
 for
$$\begin{bmatrix} y_{1} \\ y_{2} \\ y_{3} \end{bmatrix} = \begin{bmatrix} x_{1} \\ x_{2} \\ x_{1}^{2} \end{bmatrix}$$



W

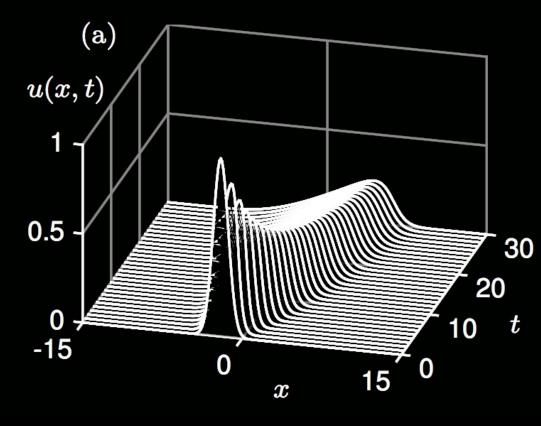


Burgers' Equation

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

Cole-Hopf

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

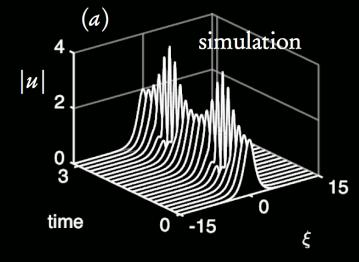


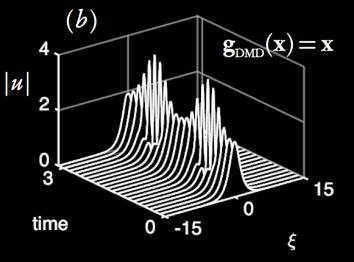
$$v_t = \epsilon v_{xx}$$

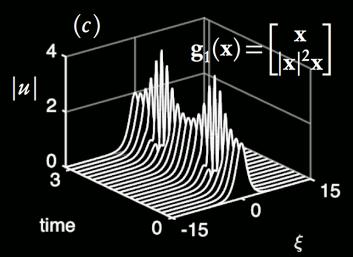
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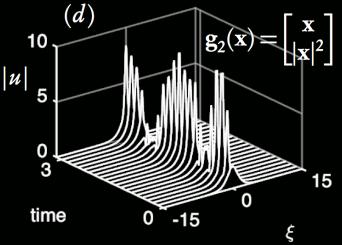
Nonlinear Schrodinger Equation

$$i\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial \xi^2} + |u|^2 u = 0$$



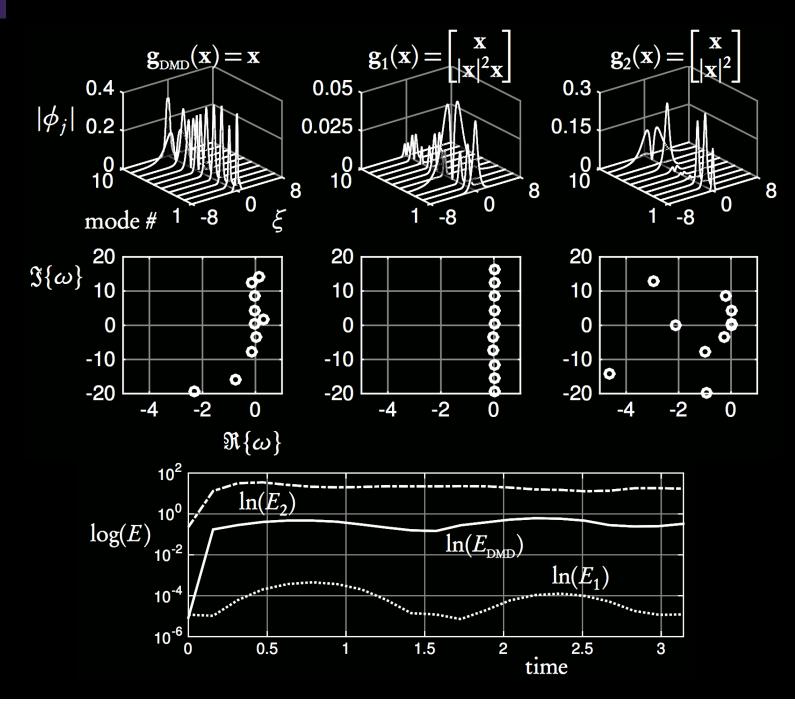




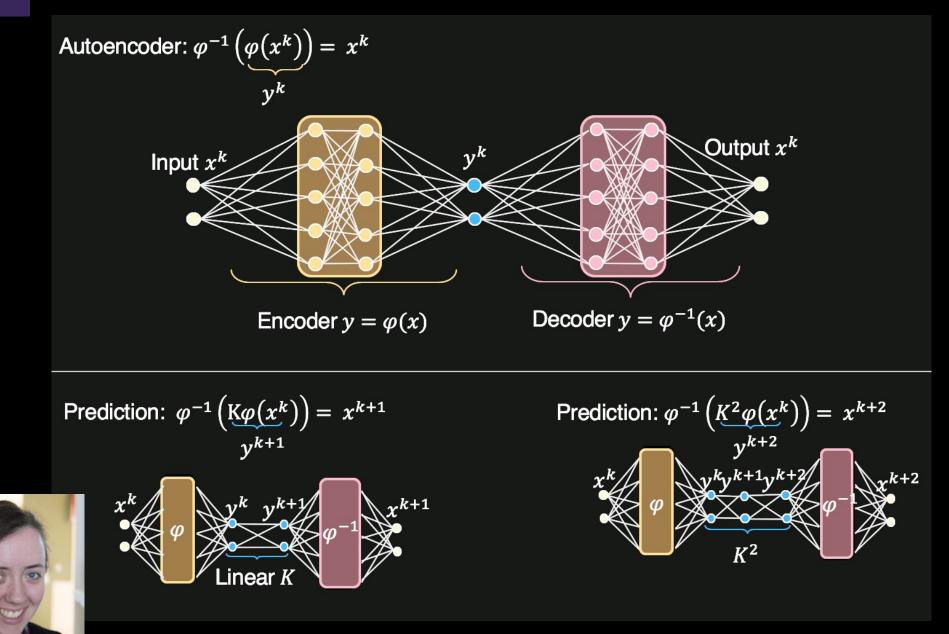




W



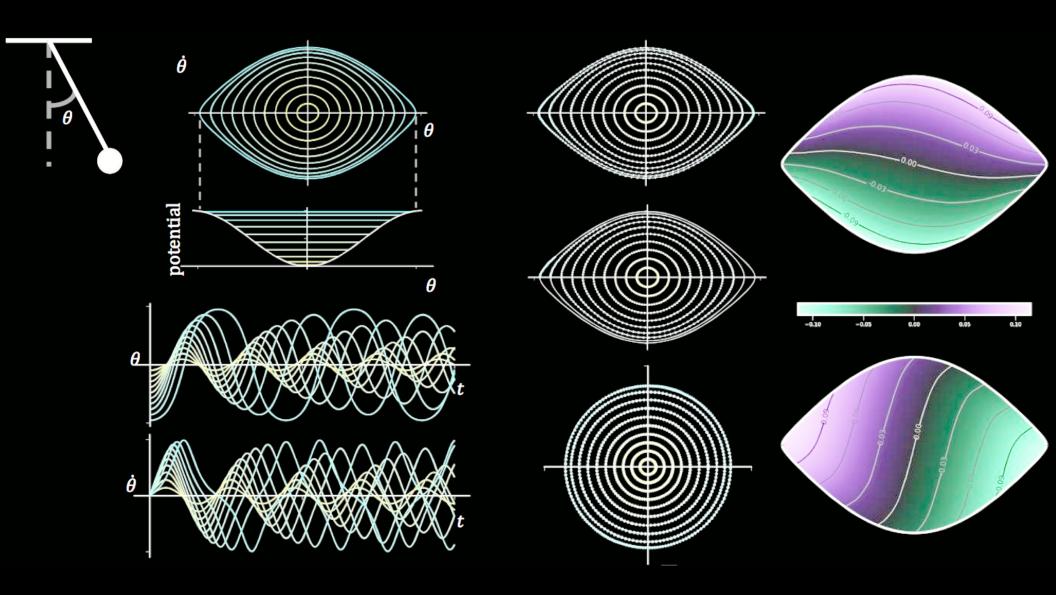
NNs for Koopman Embedding



Bethany Lusch

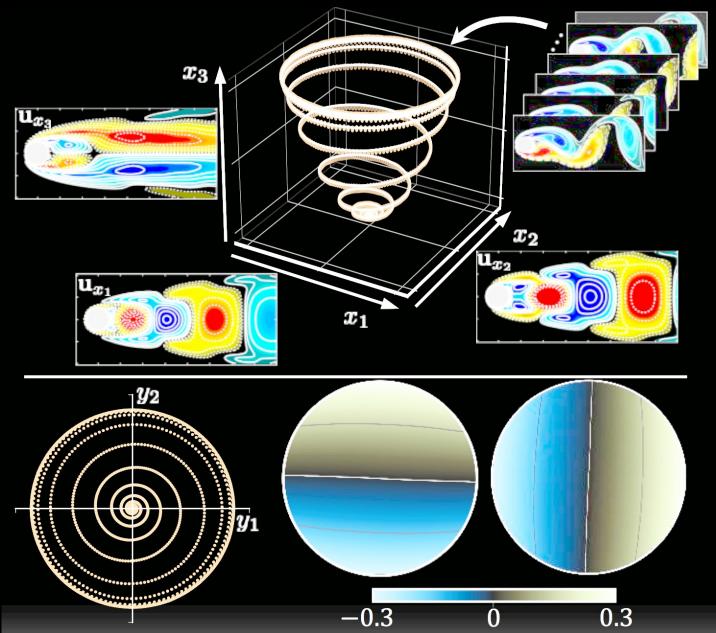


The Pendulum



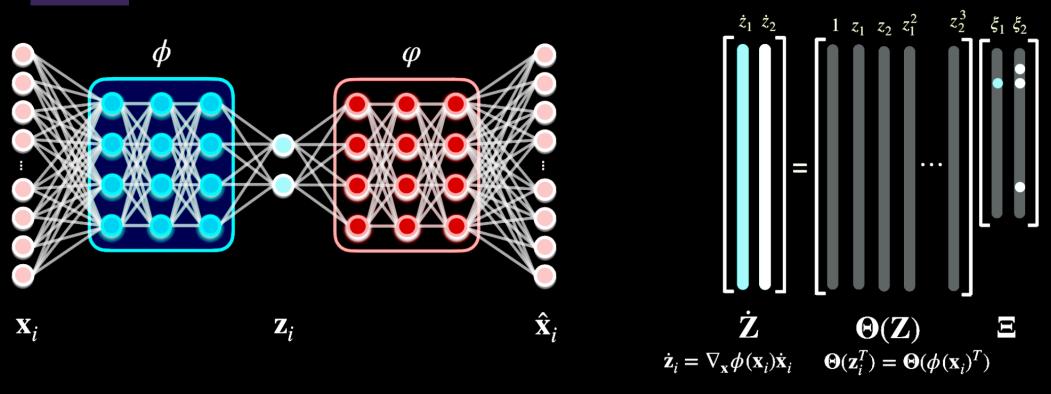
Flow Around a Cylinder

W





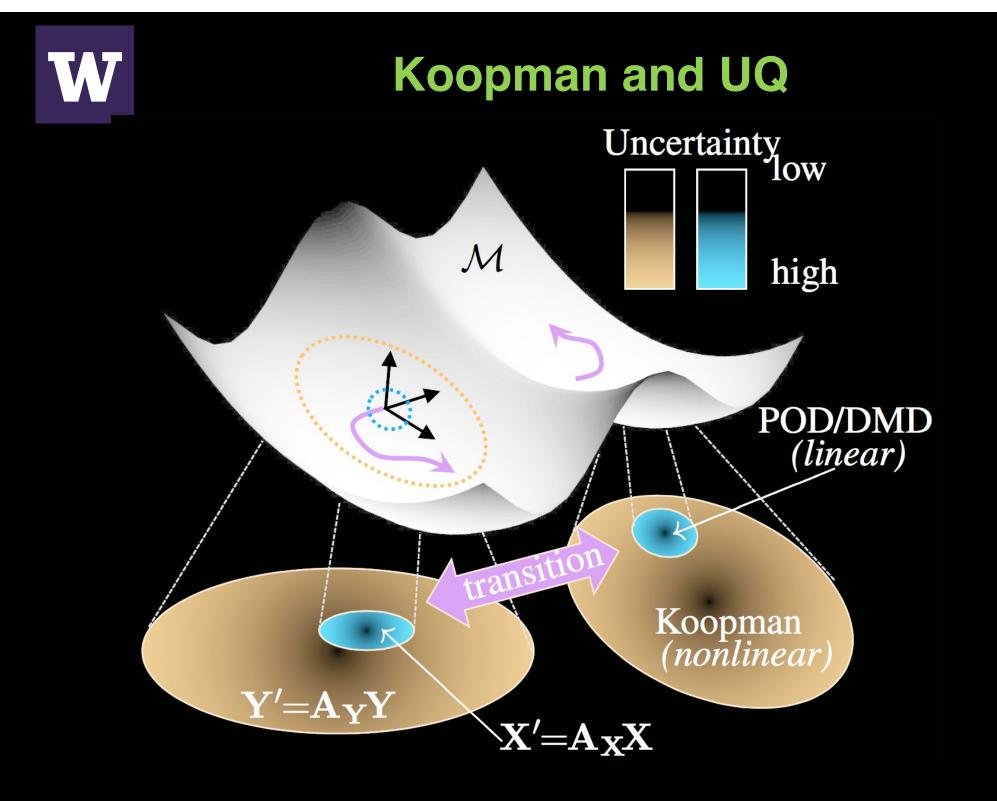
Autoencoder + SINDy



component

component



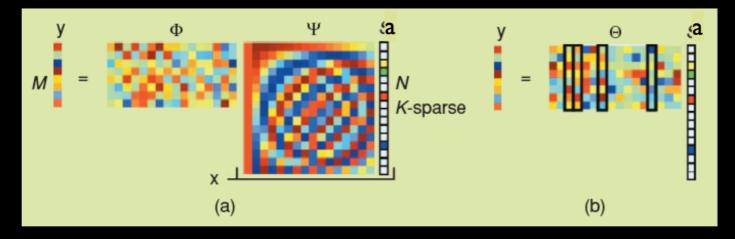




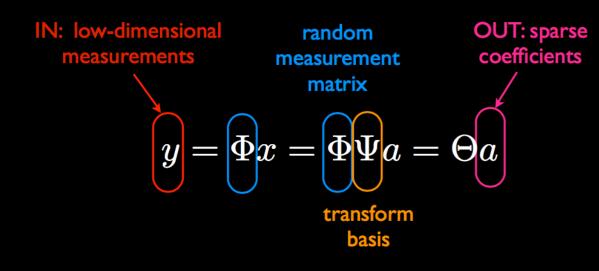
Part 3 Measurement and Sensors

Randomized Linear Algebra & Matrix Sketching

Compressive Sensing: A Cartoon



from Baraniuk, 2007.

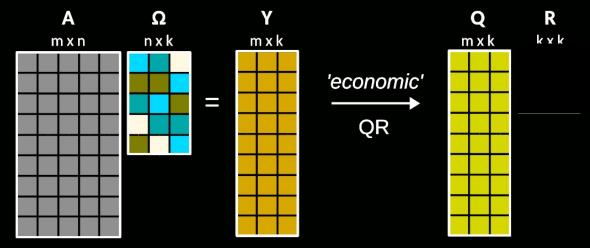


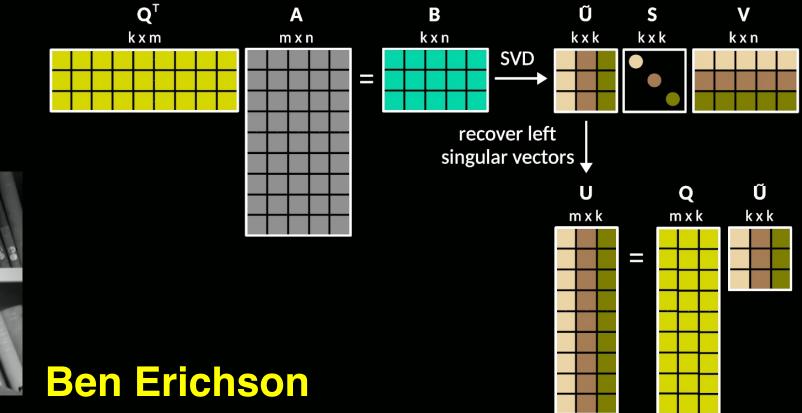
IMPORTANT: measurement matrix must be incoherent with respect to the transform basis To reconstruct: minimize $||a||_1$, such that $y = \Theta a$

Proofs by:

- Candès, Romberg & Tao, 2006.
- Donoho, 2006.

Randomized Linear Algebra







W



Gappy Methods

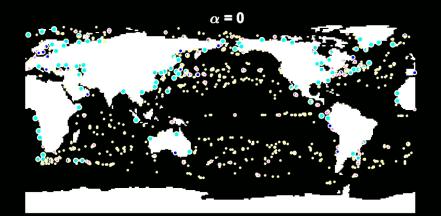
Everson & Sirovich (1995) Willcox (2005) Karniadakis co-workers (2009) Maday, Patera et al & Sorenson et al (2010, 2012) Gugerkin & Drmac (2015) Manohar, Brunton, Kutz & Brunton (2017)



Krithika Manohar

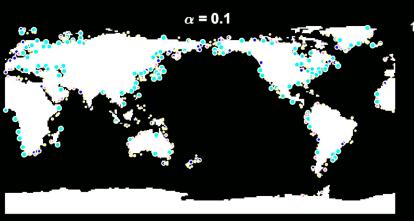
W

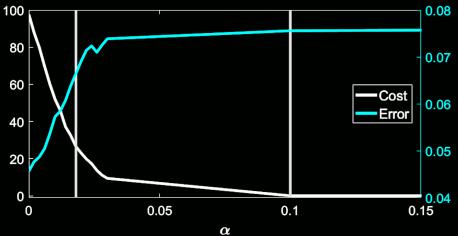
Cost with Sensors



 α = 0.018



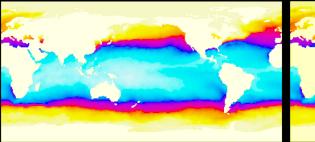


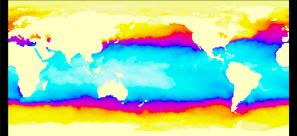


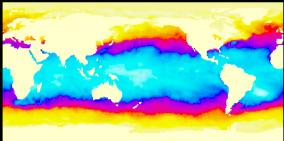
True Image

Error = 4.57%

Error = 7.87%

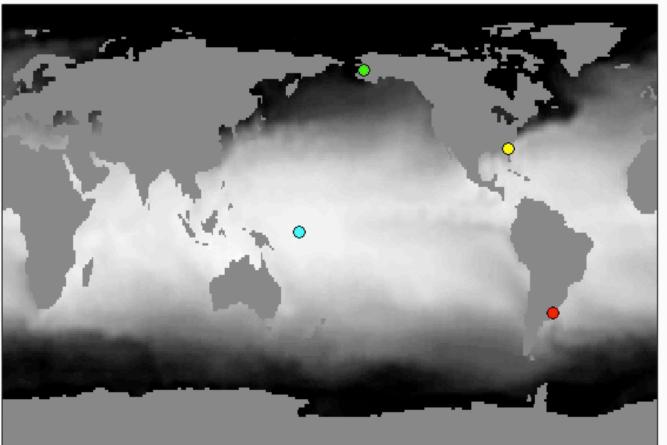


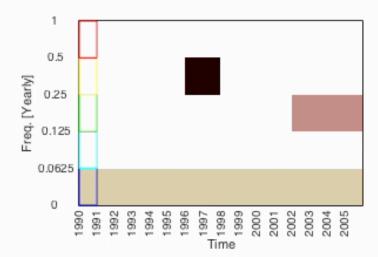


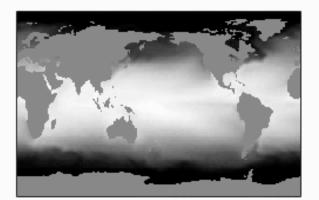


W Respect Multiscale Features

31-Dec-1989







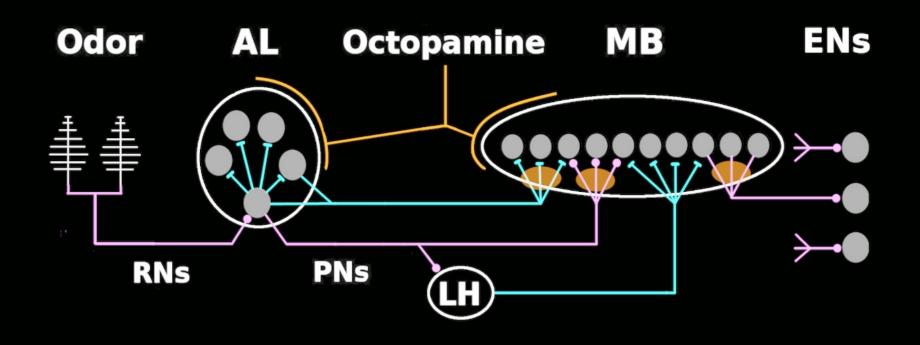


Fast Learning



Charles Delahunt

Moth Olfactory System

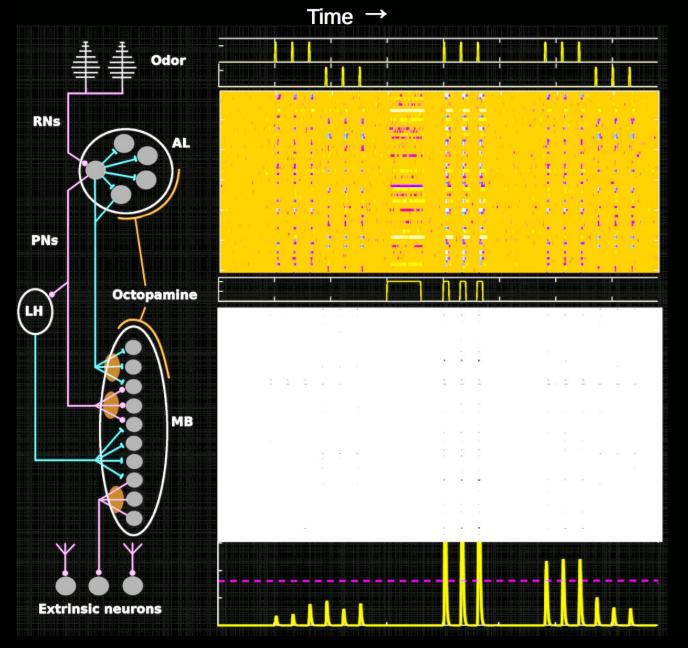


Riffell et al. Science 2013 Campbell et al. J Neuro 2013 Olson et al. Neuron 2010 Turner et al. J NeuroPhysiol 2008 Hong, Wilson. Neuron 2015

W

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

Learning New Odors



W

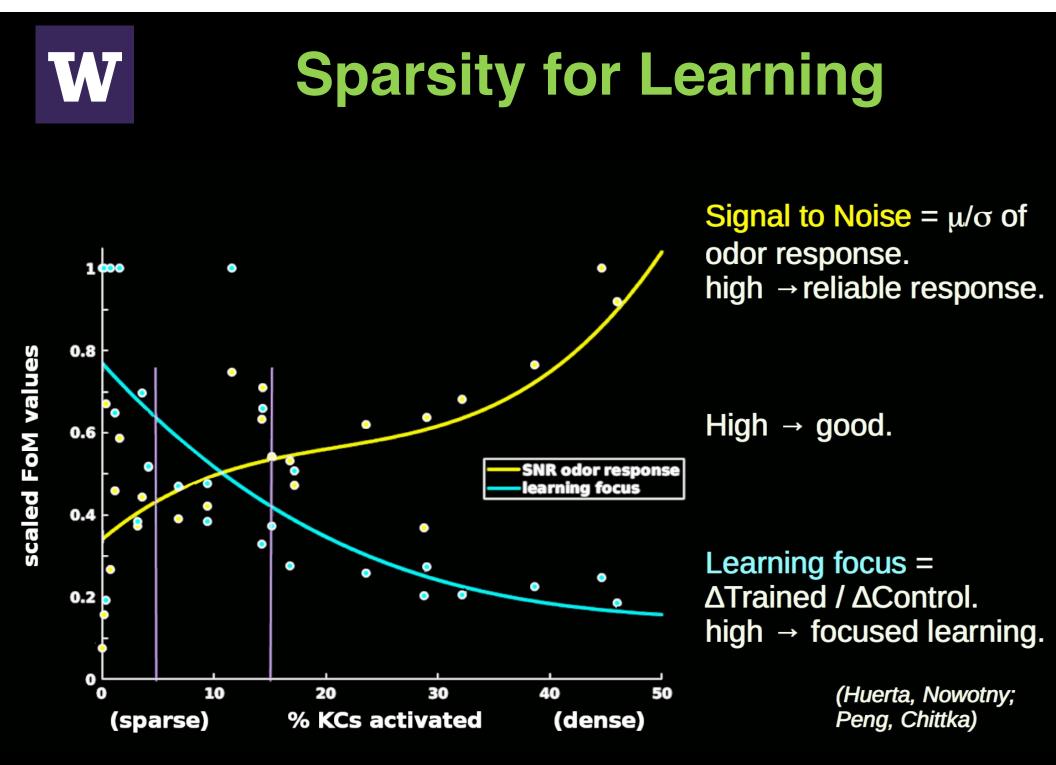
Odor inputs

AL response

Octopamine

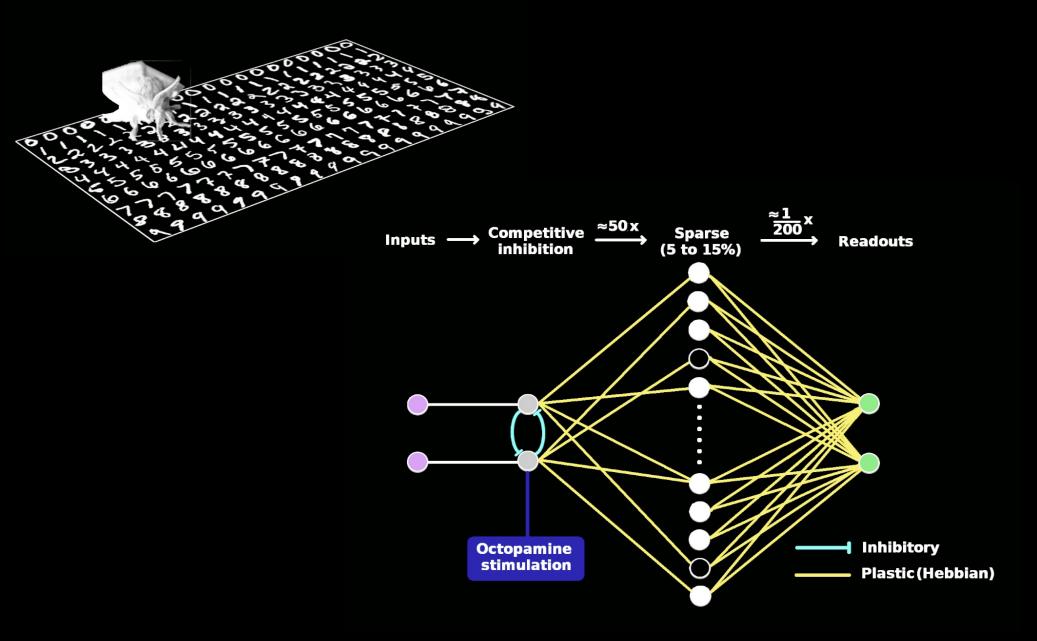
MB response

Readout neuron



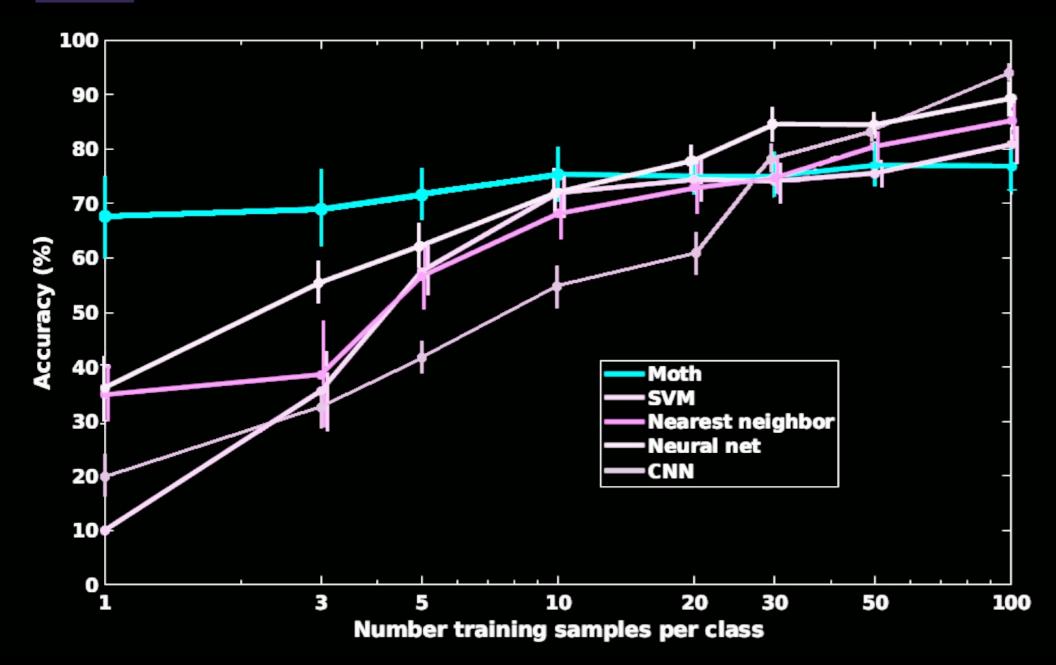
Rapid Learning in NNs

W





Comparisons

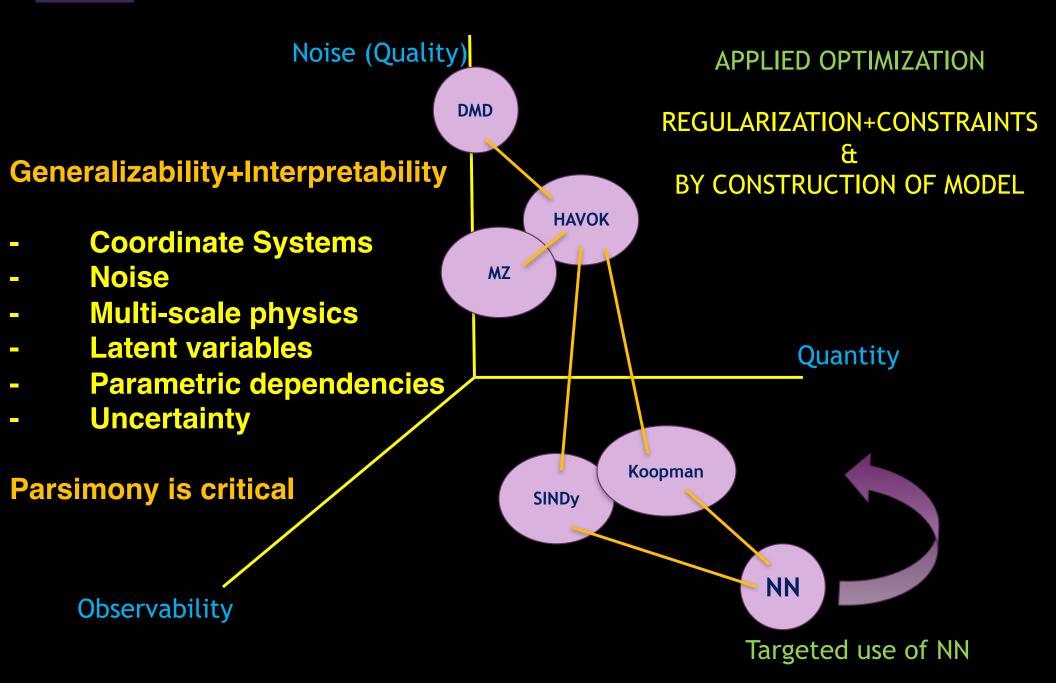




Part 4 Integration

A Diversity of Strategies

W



W

Conclusions

Model Selection & Sparse Regression Matter

- Principled approach to determining dynamics
- (i) classification, (ii) reconstruction, (iii) future state prediction
- Sensors should be maximally informative



DATA

- randomized SVD - sparse sampling - compressed sensing

Model Discovery

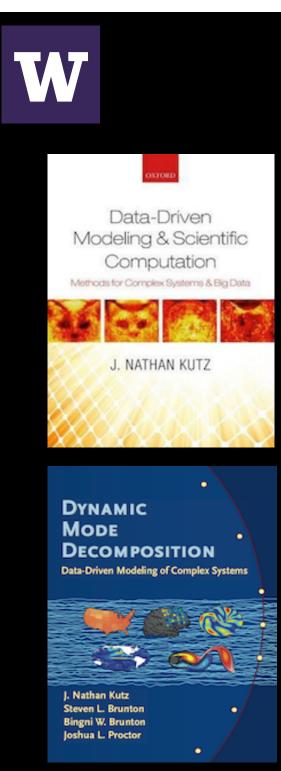
- DMD - Koopman - SINDy & PDE-FIND Prediction+Control

- ROMs

- DMDc

Koopman control

LEARNING MODULE



DATA-DRIVEN SCIENCE AND ENGINEERING

Machine Learning, Dynamical Systems, and Control

Steven L. Brunton • J. Nathan Kutz



YouTube Resources & Open Source Code

Course Structure

AMATH 563 Inferring Structure of Complex Systems

Model Selection + Background

REGRESSION

MODEL SELECTION BACKGROUND: SVD BACKGROUND:

BACKGROUND: CLASSIFICATION +

OPTIMIZATION

Dynamics + Discovery

MODEL DISCOVERY DATA ASSIMILATION DMD + KOOPMAN THEORY + EMBEDDING Learning + Feature Extraction

NEURAL NETWORKS + DEEP LEARNING

RANDOMLIZED LINEAR ALGEBRA

MULTI-RESOLUTION ANALYSIS + WAVELETS

Networks + Inference

NETWORK CONCEPTS

INFERENCE + CAUSALITY PROBABILISTIC GRAPHICAL MODELS

Inferring Structure of Complex Systems

Homework + Data

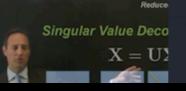
Homework 1 | DATA Homework 2 | PDECODES

About This Course

This webpage is designed as the primary source of lectures, notes, codes and data for AMATH 563: Inferring Structure Of Complex Systems.

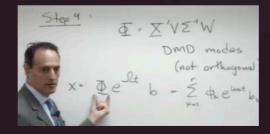
Topics Covered

- Week 1: Model selection and regression
- Week 2: Model discovery
- Week 3: Data Assimilation



Online Materials

Lecture 1



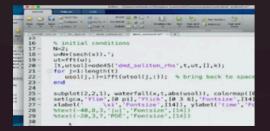
[Part 1] [Part 2]

Dynamic Mode Decomposition: This lecture provides an introduction to the Dynamic Mode Decomposition (DMD). The focus is on approximating a nonlinear dynamical system with a linear system.

MATLAB CODE

dmd_intro.m

Lecture 2



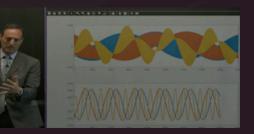
[view]

Koopman Theory: This lecture generalizes the DMD method to a function of the state-space, thus potentially providing a coordinate system that is intrinsically linear.

MATLAB CODE

- dmd_soliton.m
- dmd_soliton_rhs.m

Lecture 3



[view]

Time-Delay Embeddings: This lecture generalizes the Koopman/DMD method to a function of the state-space created by time-delay embedding of the dynamical trajectories.

MATLAB CODE

- time_delay.m
- rhs_dyn.m

KEY REFERENCES AND SUPPLEMENTARY VIDEOS



Koopman observable subspaces and finite linear representations of nonlinear dynamical systems for control

This video highlights the recent innovation of Koopman analysis for representing nonlinear systems and control. [Part 1], [Part 2], [Part 3]

 S. L. Brunton, B. Brunton, J. L. Proctor and J. N. Kutz, Koopman observable subspaces and finite linear representations of nonlinear dynamical systems for control PLOS ONE (2016)



Math is Awesome