Machine Learning *Dynamical Systems* from *Data*

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What's ***data***? What's ***learning dynamical systems*** ?

- (1) Data representation
  - Video
    - Extract only physically relevant variables, drop others [1][12]
    - Disentangle physics and shape factors [2][3]
  - Low-dim physical trajectory [4] → Good!
  - High-dim physical trajectory/fields
    - Collective coordinate: [5][16]
    - Quantization of particles/supercells: Perception + GNN [6][13][14]
    - Renormalizing flow [?Multi-scale models]

Combination & Interplay

- (2) Learning goal
  - Equation
    - Sparse regression [5]
    - Recurrent neural models [1][2]
    - Symbolic regression
      - First numeric, then symbolic [6]
      - Numeric-symbolic hybrid system [15]
  - Pattern
    - Bifurcation diagram [7][8]
    - Conservation Law, Symmetry [10][11][12]
    - Periodic orbit, regular-chaotic phase transition [9]

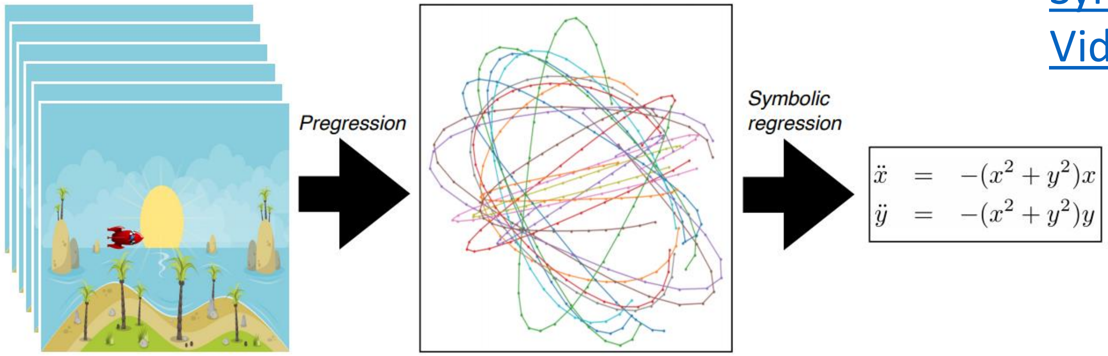
help

Papers

- [1] Symbolic Pregression: Discovering Physical Laws from Distorted Video
- [2] Disentangling Physical Dynamics from Unknown Factors for Unsupervised Video Prediction
- [3] Contrastive Learning of Structured World Models
- [4] Toward an AI Physicist for Unsupervised Learning
- [5] Data-driven discovery of coordinates and governing equations
- [6] Discovering Symbolic Models from Deep Learning with Inductive Biases
- [7] Inferring Global Dynamics Using a Learning Machine
- [8] Reconstruction of normal forms by learning informed observation geometries from data
- [9] AI Poincare (In preparation)
- [10] Lagrangian Neural Network
- [11] Hamiltonian Neural Network
- [12] Hamiltonian Generative Networks
- [13] Vortex Net: Learning Complex Dynamics Systems with Physics-Embedded Networks
- [14] Coarse-graining auto-encoders for molecular dynamics
- [15] Integration of Neural Network-Based Symbolic Regression in Deep Learning for Scientific Discovery
- [16] Neural Canonical Transformation with Symplectic Flows
- [17] PDE-net: Learning PDE from data

Data Representation

Video



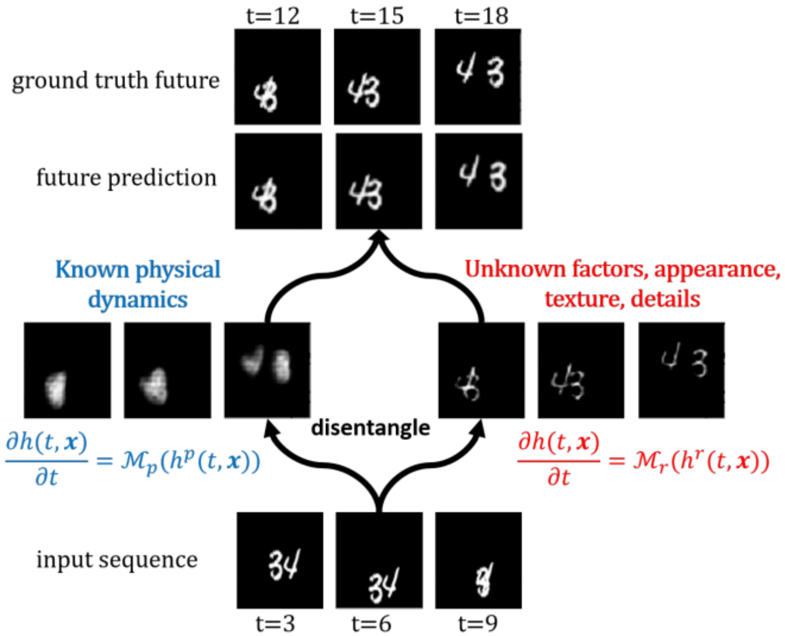
[Symbolic Pregression: Discovering Physical Laws from Distorted Video](#)

[1] A rocket in motion with static background

Target:

(1) Finding a low-dim physical latent space

(2) Finding symbolic dynamical equations in the latent space



[Disentangling Physical Dynamics from Unknown Factors for Unsupervised Video Prediction](#)

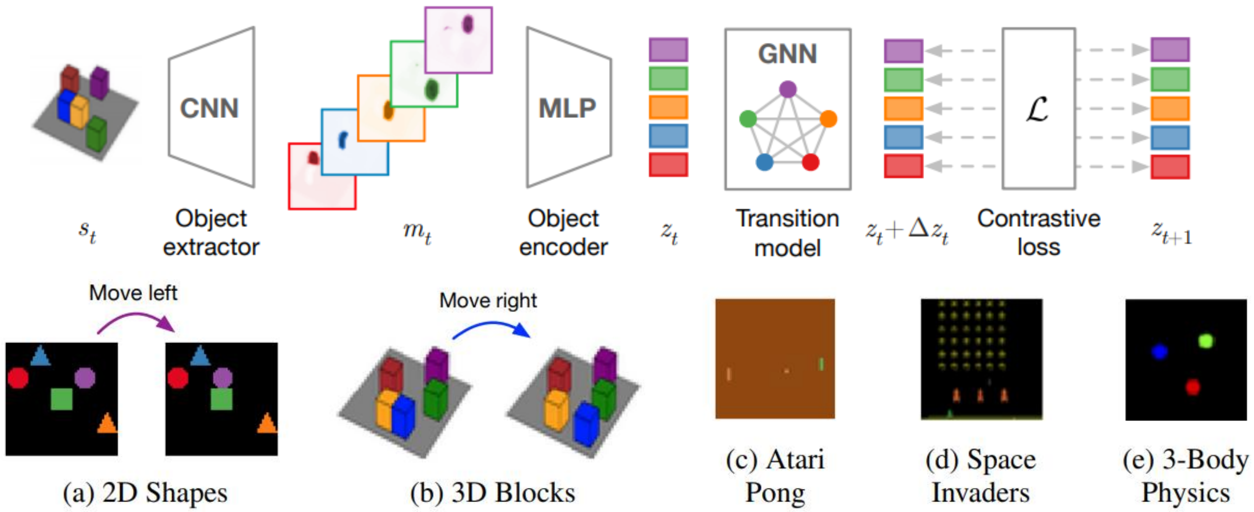
[2] Two MNIST digits are moving in the bounded frame

Target:

(1) Disentangling physical factors and shape factors

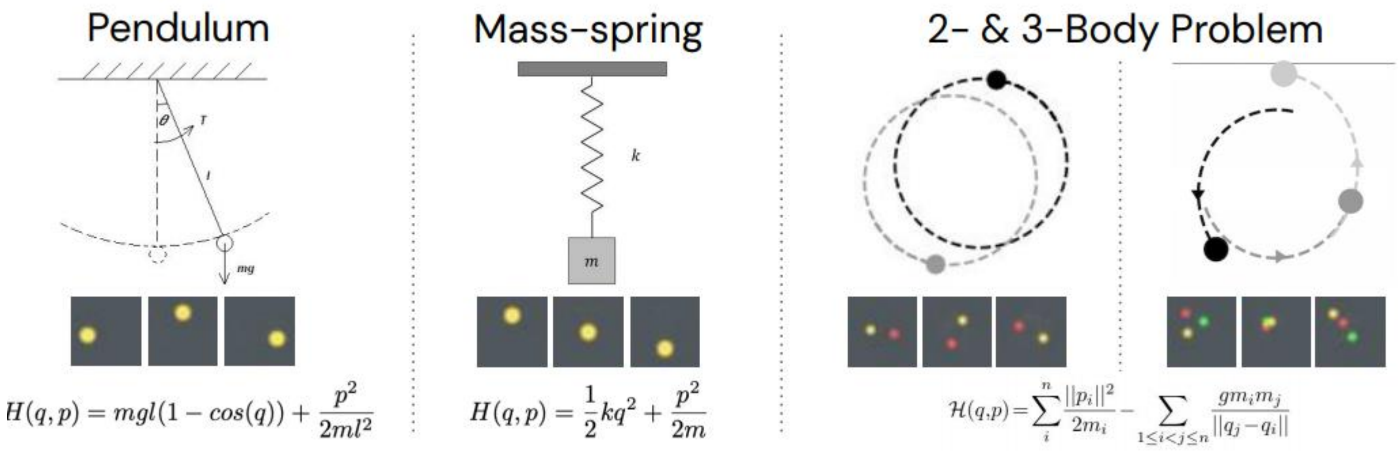
(2) Finding dynamics for both physical and shape factors

Video



[Contrastive Learning of Structured World Models]()

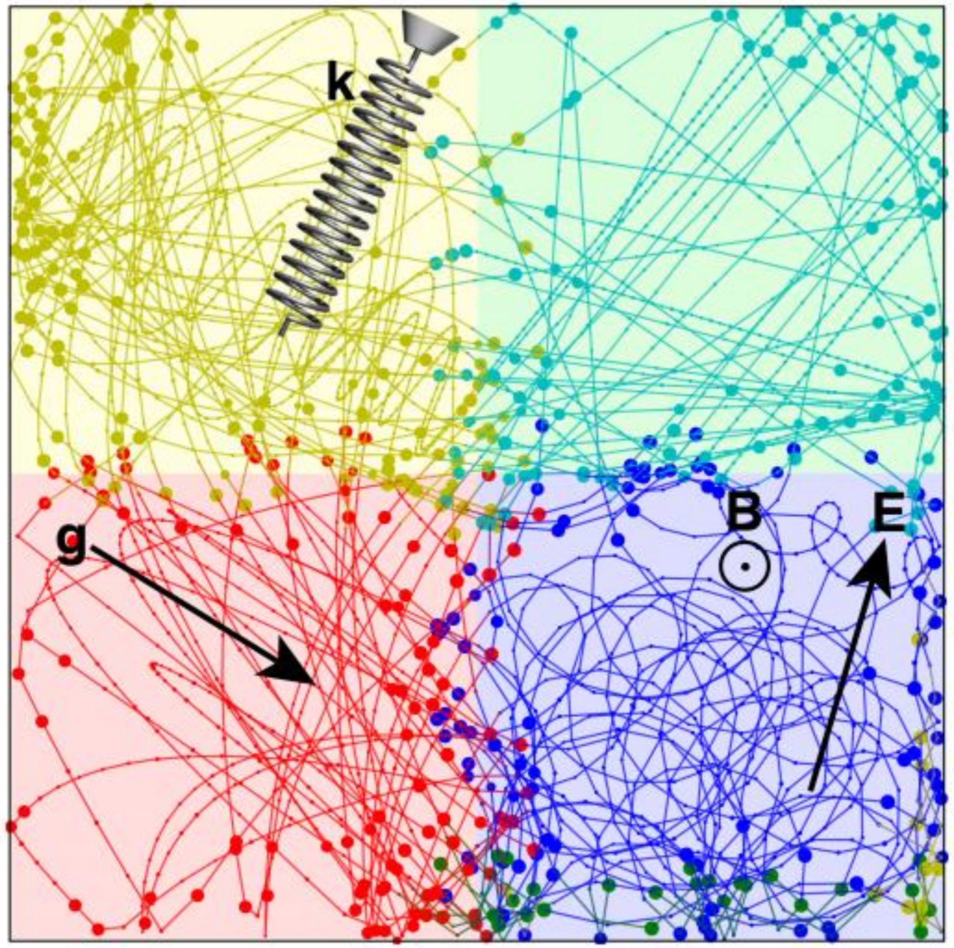
[3] Multiple objects, Games
Target:
(1) Finding latent space for state and action
(2) Learning transition model (dynamics)



[Hamiltonian Generative Networks]()

[12] N-body in motion
Target:
(1) Finding latent space for state
(2) Learning dynamics (inductive bias: Hamiltonian dynamics)

Low-dim trajectory



[Toward an AI Physicist for Unsupervised Learning]

[4] Position and momentum/velocity
Target:
(1) Learn different theories (dynamics)
(2) Unify & Classify theories

High-dim space

[5] Target:

(1) Learn latent space

(2) Find dynamical equation in latent space

[Data-driven discovery of coordinates and governing equations]

(a) Lorenz System (ODE-> Embed in high-dim space)

$$\dot{z}_1 = \sigma(z_2 - z_1) \quad (8a)$$
$$\dot{z}_2 = z_1(\rho - z_3) - z_2 \quad (8b)$$
$$\dot{z}_3 = z_1 z_2 - \beta z_3. \quad (8c)$$

The dynamics of the Lorenz system are chaotic and highly nonlinear, making it an ideal test problem for model discovery. To create a high-dimensional data set based on this system, we choose six fixed spatial modes $\mathbf{u}_1, \ldots, \mathbf{u}_6 \in \mathbb{R}^{128}$, given by Legendre polynomials, and define

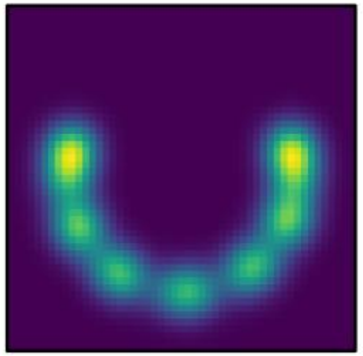
$$\mathbf{x}(t) = \mathbf{u}_1 z_1(t) + \mathbf{u}_2 z_2(t) + \mathbf{u}_3 z_3(t) + \mathbf{u}_4 z_1(t)^3 + \mathbf{u}_5 z_2(t)^3 + \mathbf{u}_6 z_3(t)^3. \quad (9)$$

(b) Reaction-Diffusion System (PDE, high-dim in nature)

$$u_t = (1 - (u^2 + v^2))u + \beta(u^2 + v^2)v + d_1(u_{xx} + u_{yy}) \quad (10a)$$
$$v_t = -\beta(u^2 + v^2)u + (1 - (u^2 + v^2))v + d_2(v_{xx} + v_{yy}) \quad (10b)$$

with $d_1, d_2 = 0.1$ and $\beta = 1$. This set of equations generates a spiral wave formation, whose behavior can be approximately captured by two oscillating spatial modes. We apply our method to snapshots of $u(x, y, t)$ generated by the above equations. Snapshots are collected at discretized points of the xy-domain, resulting in a high-dimensional input data set with $n = 10^4$.

(c) Nonlinear pendulum (ODE->video)

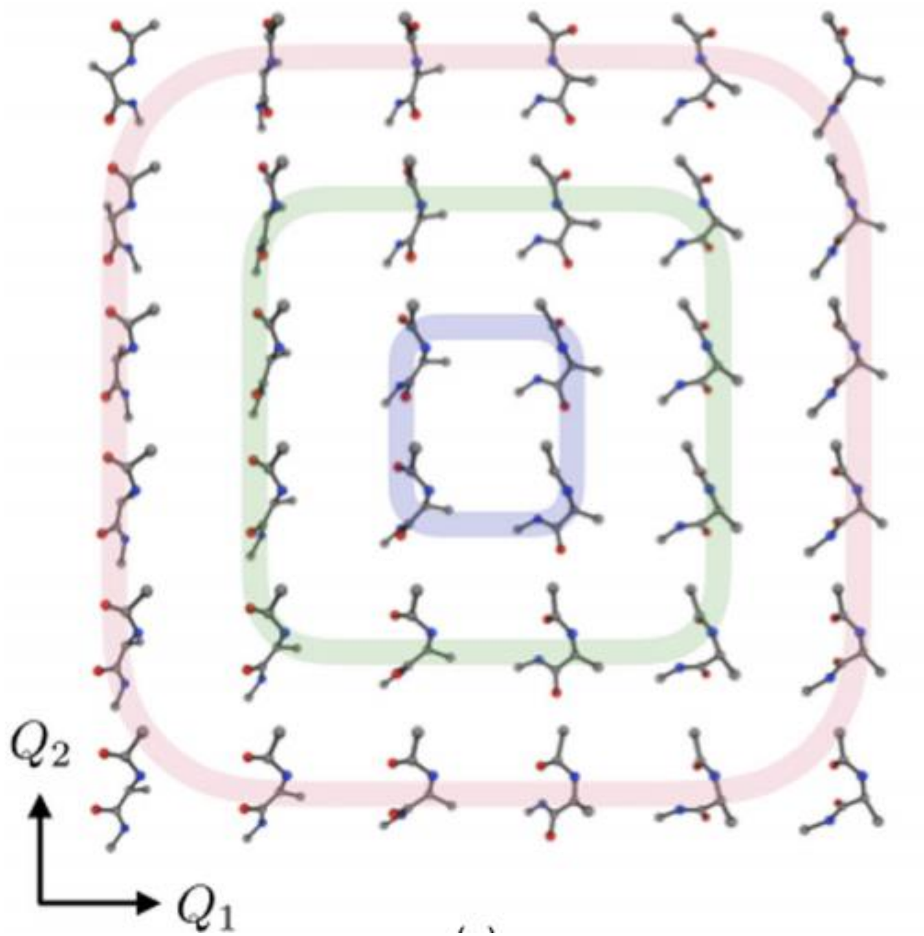


$$\ddot{z} = -0.99 \sin z$$

High-dim space

[16] Target:
(1) Learn (possibly nonlinear) slow modes
(2) Hamiltonian in latent space are as simple as (decoupled) harmonic oscillators

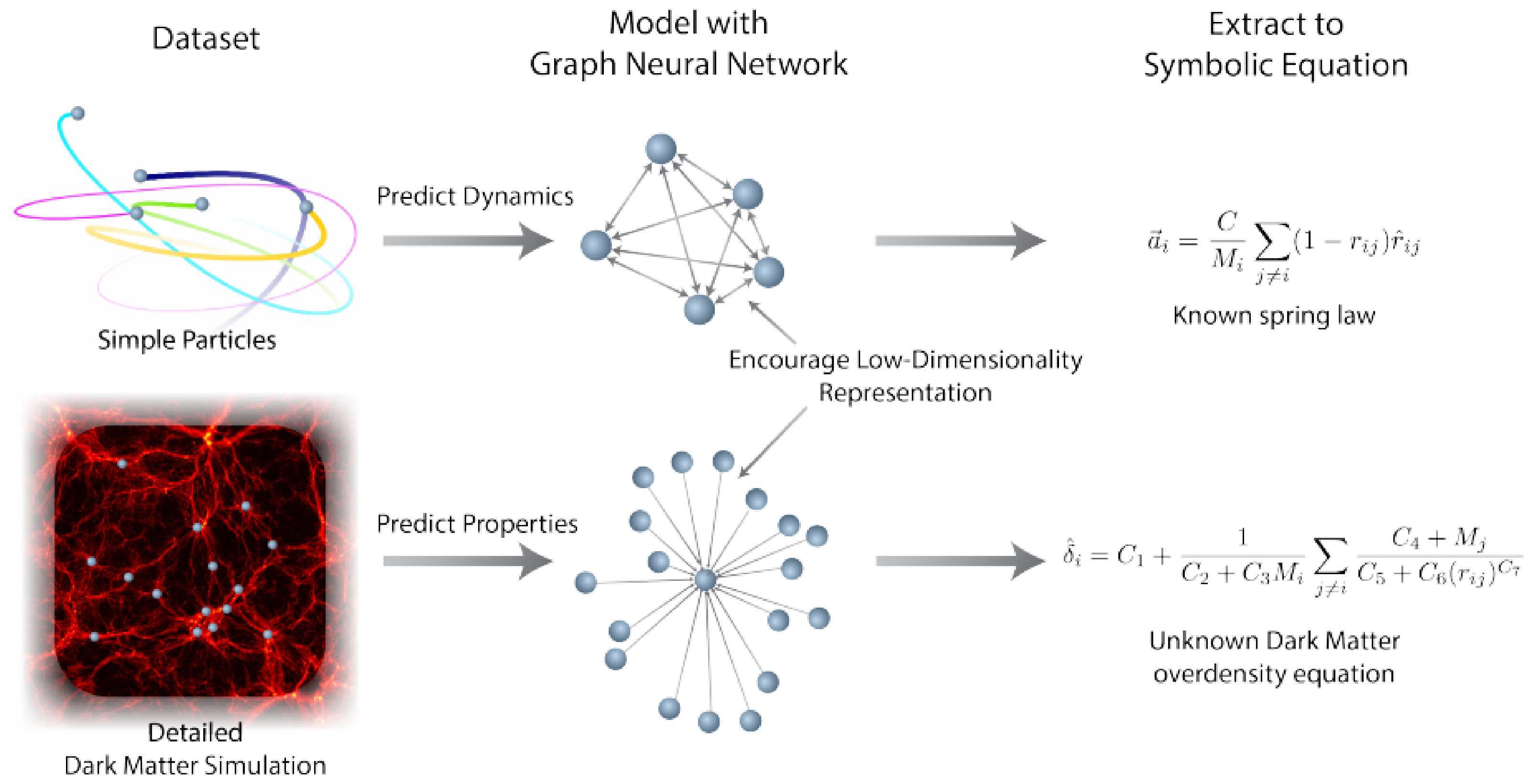
[Neural Canonical Transformation with Symplectic Flows]



High-dim space

[6] Target:
(1) Learn particle representation of field
(2) Learn interactions between particles
(GNN) -> N-body dynamics

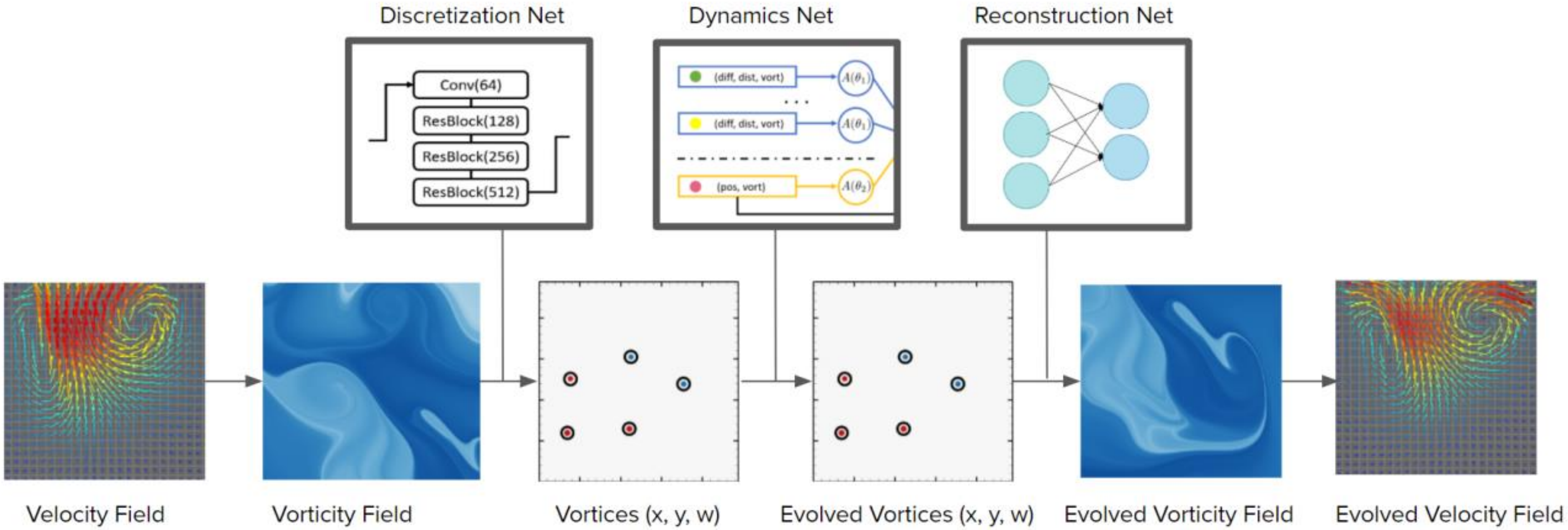
[Discovering Symbolic Models from Deep Learning with Inductive Biases]()



High-dim space

[13] Target:
(1) Fluid -> vortices -> Fluid
(2) Learn dynamics of vortices (GNN)

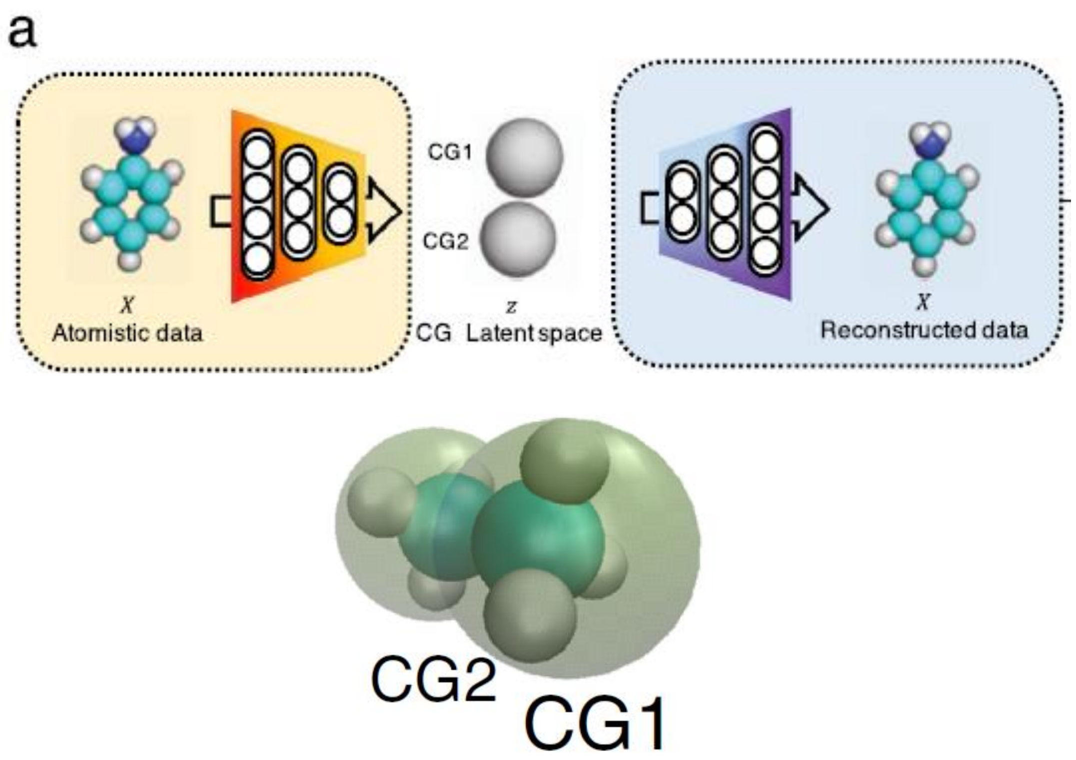
[Vortex Net: Learning Complex Dynamics Systems with Physics-Embedded Networks]

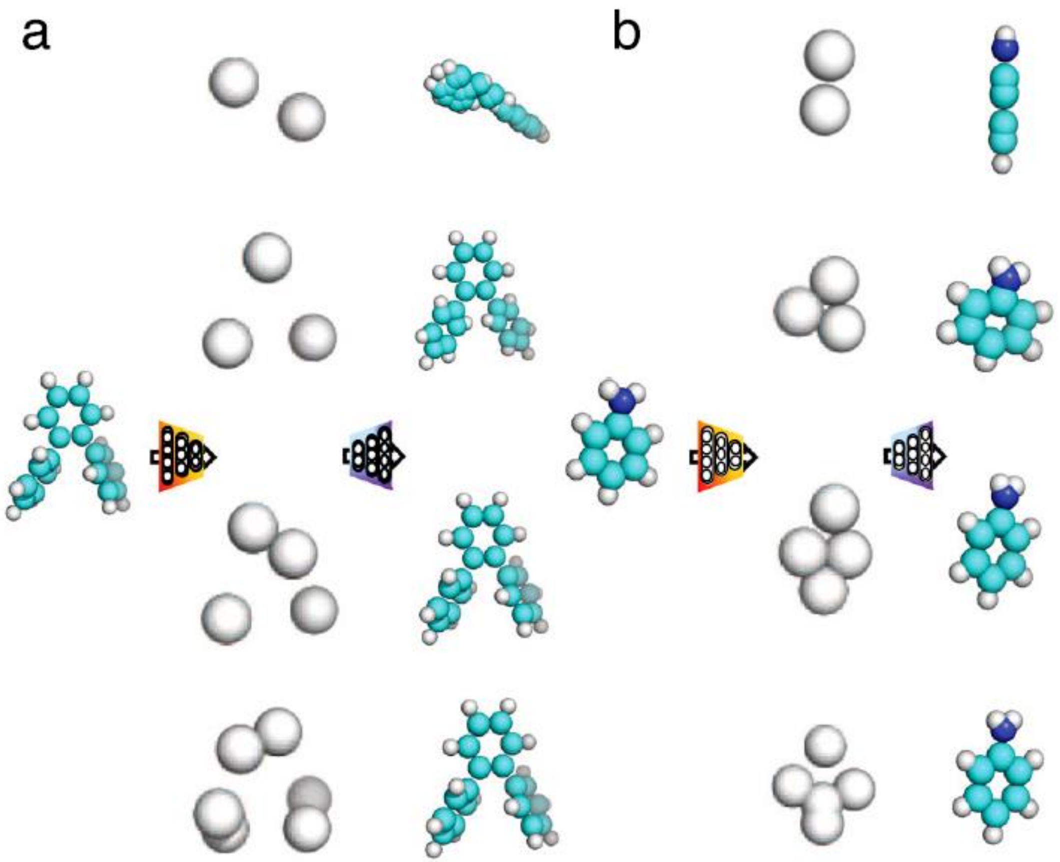


High-dim space

[Coarse-graining auto-encoders for molecular dynamics]

[14] Target:
(1) Learn to partition atoms to "super-atoms"
(2) Learn dynamics for "super-atoms"





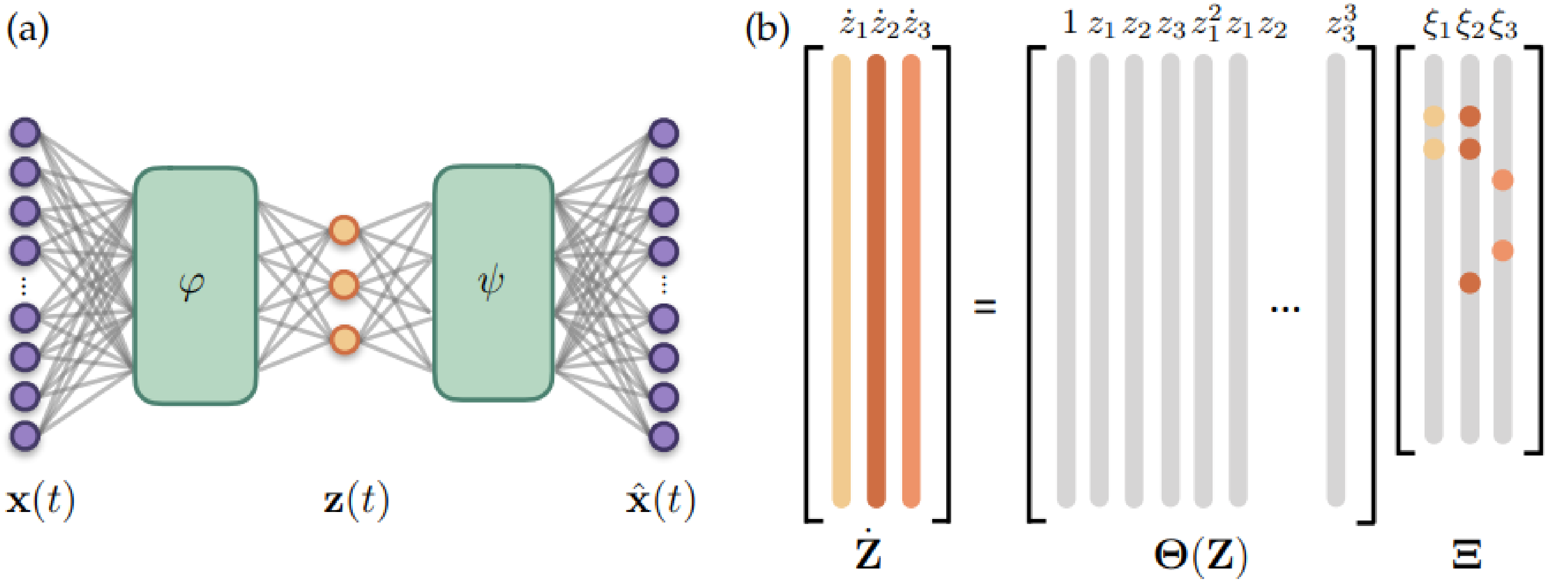
Learning Goal

Equation: Sparse Regression

[5] sparse identification of nonlinear dynamics (SINDY)

[Data-driven discovery of coordinates and governing equations]

Idea: (1) The dynamics in latent space comes from a (finite) library;
(2) All terms in the library are pre-computed for each time point and then perform sparse regression



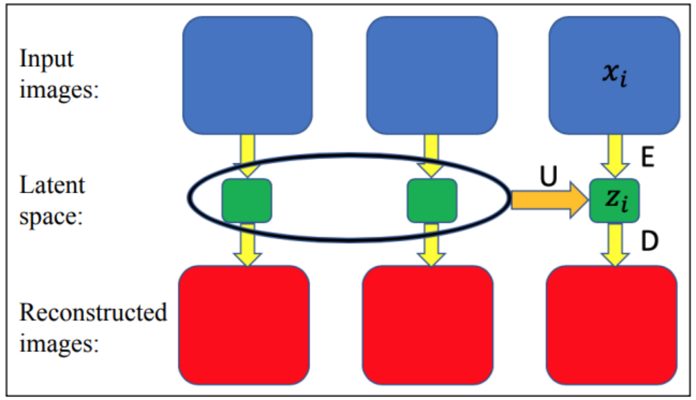
$\dot{\mathbf{z}}_i = \nabla_{\mathbf{x}} \varphi(\mathbf{x}_i) \dot{\mathbf{x}}_i \qquad \mathbf{\Theta}(\mathbf{z}_i^T) = \mathbf{\Theta}(\varphi(\mathbf{x}_i)^T)$

$$\underbrace{\|\mathbf{x} - \psi(\mathbf{z})\|_2^2}_{\text{reconstruction loss}} + \lambda_1 \underbrace{\left\|\dot{\mathbf{x}} - (\nabla_{\mathbf{z}}\psi(\mathbf{z}))\left(\mathbf{\Theta}(\mathbf{z}^T)\mathbf{\Xi}\right)\right\|_2^2}_{\text{SINDy loss in } \dot{\mathbf{x}}} + \lambda_2 \underbrace{\left\|(\nabla_{\mathbf{x}}\mathbf{z})\,\dot{\mathbf{x}} - \mathbf{\Theta}(\mathbf{z}^T)\mathbf{\Xi}\right\|_2^2}_{\text{SINDy loss in } \dot{\mathbf{z}}} + \lambda_3 \underbrace{\|\mathbf{\Xi}\|_1}_{\substack{\text{SINDy} \\ \text{regularization}}}$$

Equation: Recurrent neural models

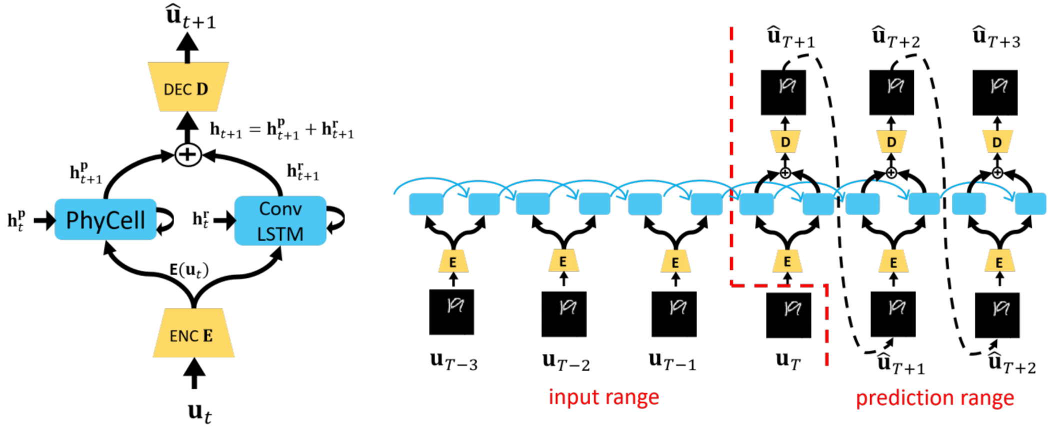
[Symbolic Pregression: Discovering Physical Laws from Distorted Video]

[1] Learning symbolic physical law from raw distorted videos



[Disentangling Physical Dynamics from Unknown Factors for Unsupervised Video Prediction]

[2] Learning Moving MNIST by disentangling physical and shape factors



(a) PhyDNet disentangling recurrent bloc **(b) Global seq2seq architecture**

[17] PDE-net

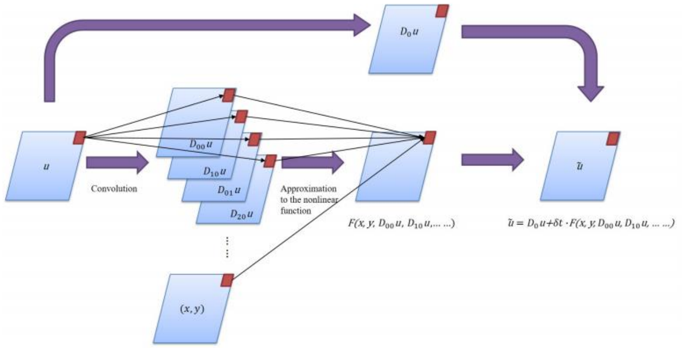
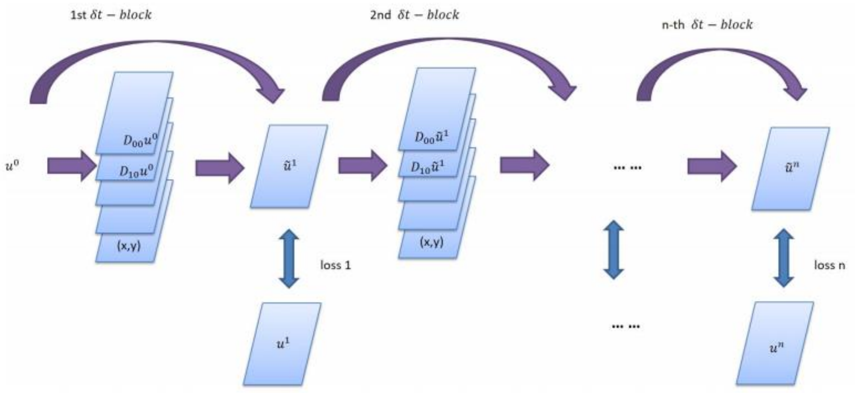


Figure 1: The schematic diagram of a δt-block.

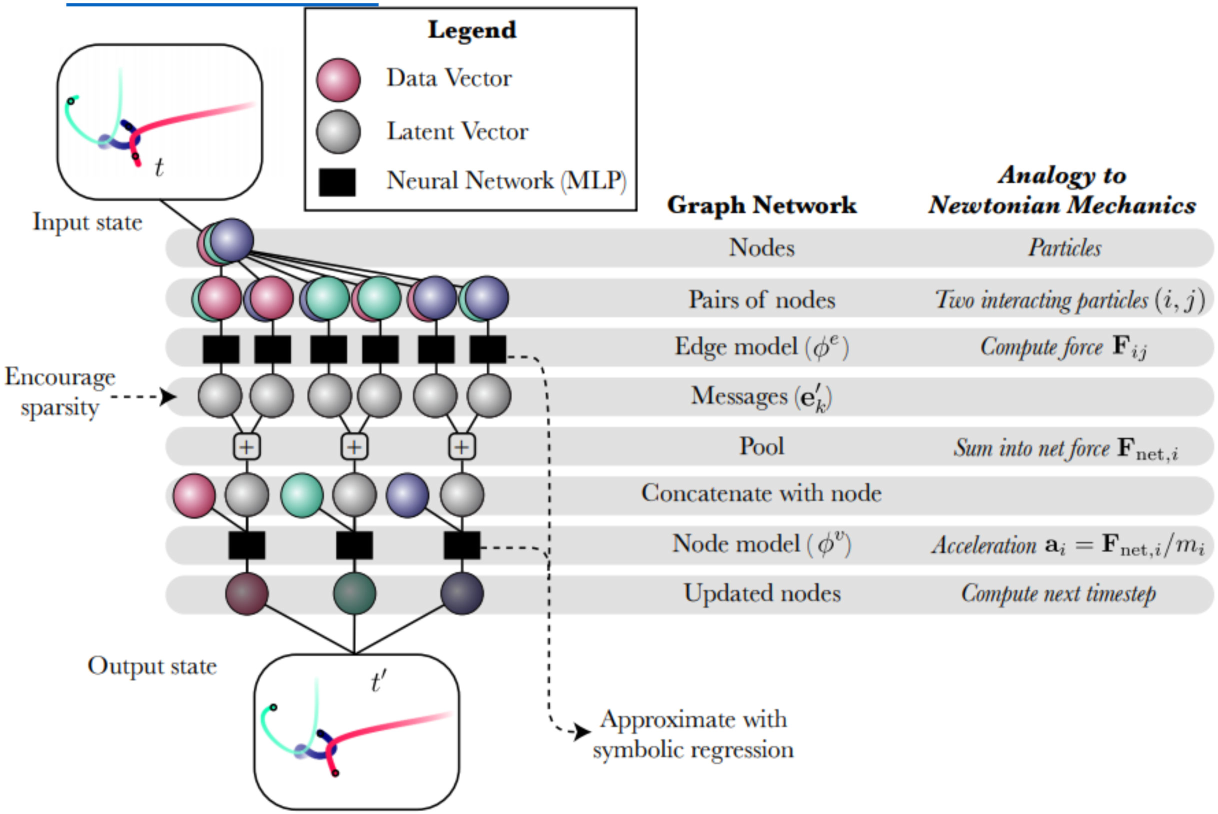


[PDE-net: Learning PDE from data]

Equation: Symbolic regression

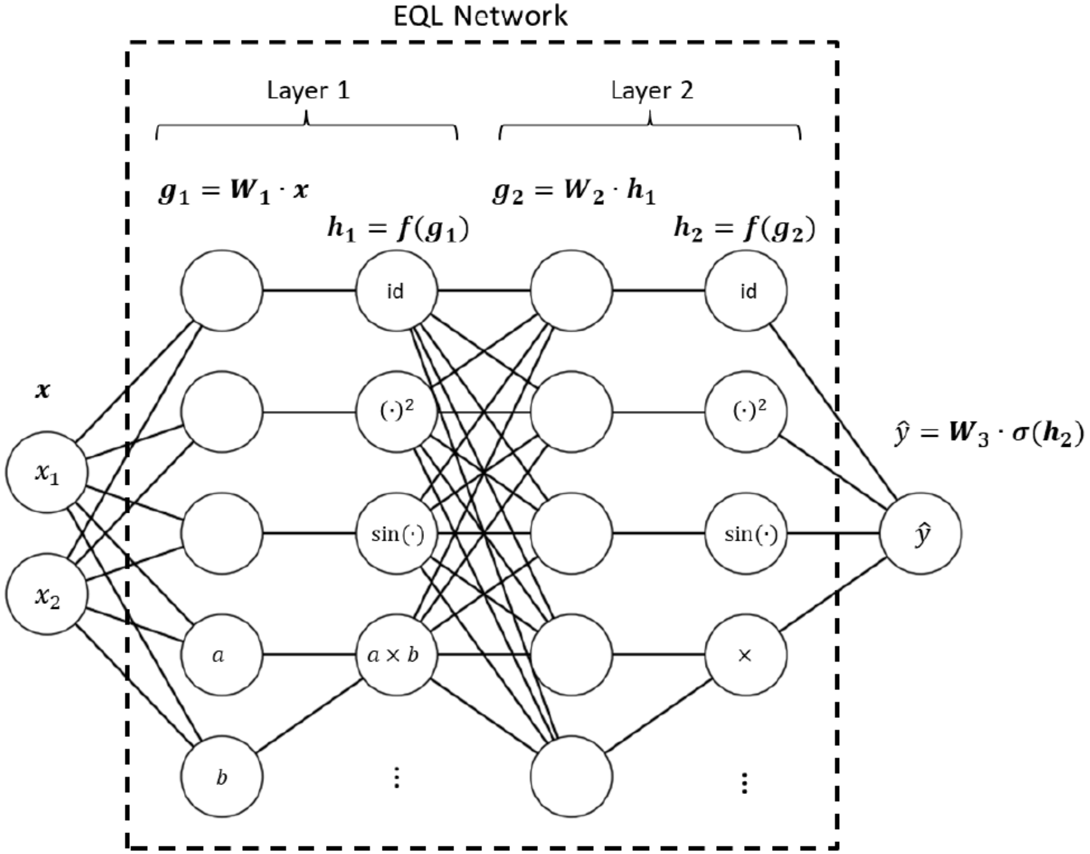
[6] First numeric, then symbolic

Discovering Symbolic Models from Deep Learning with Inductive Biases



[15] Neural-symbolic hybrid system

Integration of Neural Network-Based Symbolic Regression in Deep Learning for Scientific Discovery



Pattern: Bifurcation Diagram

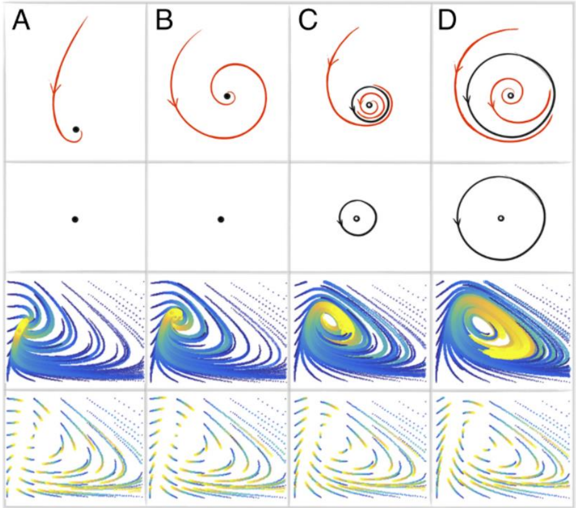
[Inferring Global Dynamics Using a Learning Machine](#)

[7] Learning Bogdanov-Takens bifurcation map

As an illustrative example, consider the following dynamical system, arising in the unfolding of the Bogdanov–Takens singularity (20):

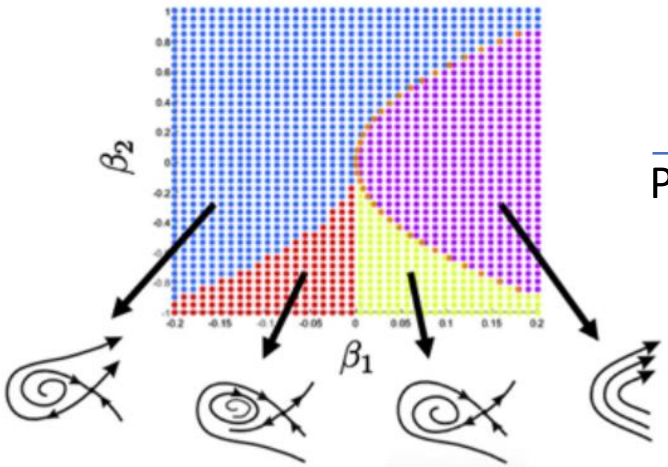
$$\frac{dx_1}{dt} = x_2$$
$$\frac{dx_2}{dt} = \beta_1 + \beta_2 x_1 + x_1^2 - x_1 x_2. \qquad \textbf{[3]}$$

Human beings can discover bifurcation with raw eyes.



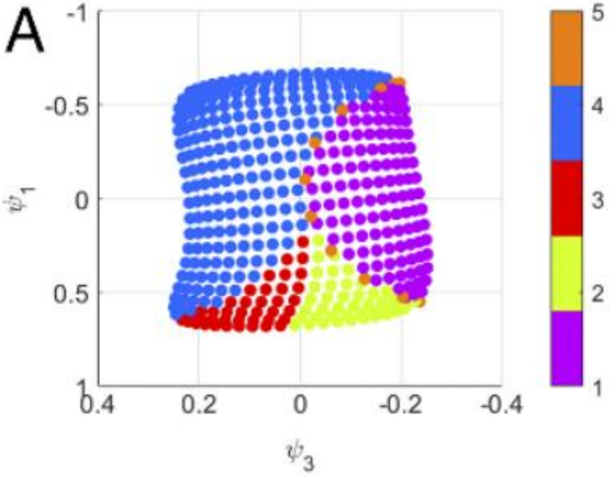
Increasing difficulty

Ground Truth



Clustering

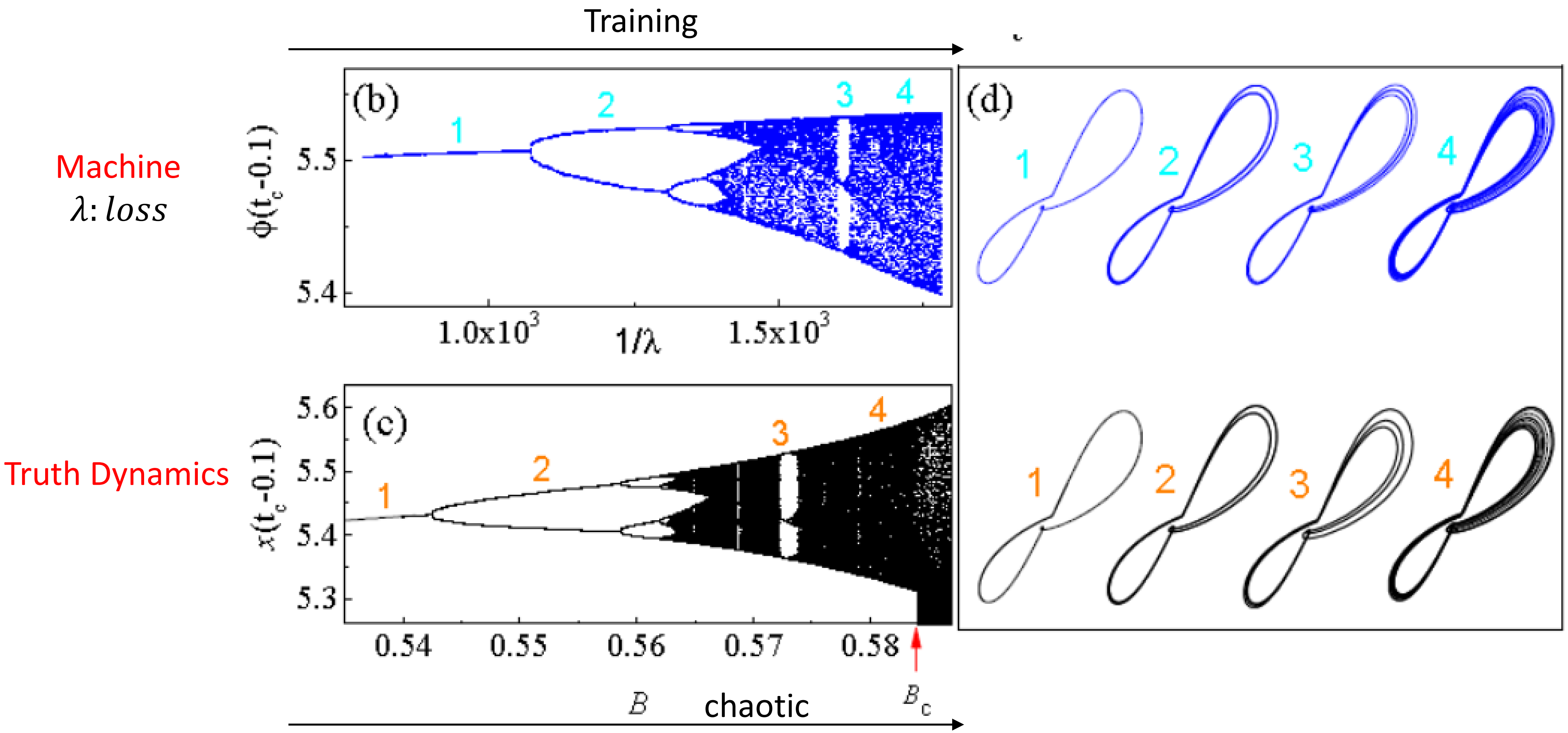
Phase <-> Cluster



Pattern: Bifurcation Diagram

Reconstruction of normal forms by learning informed observation geometries from data

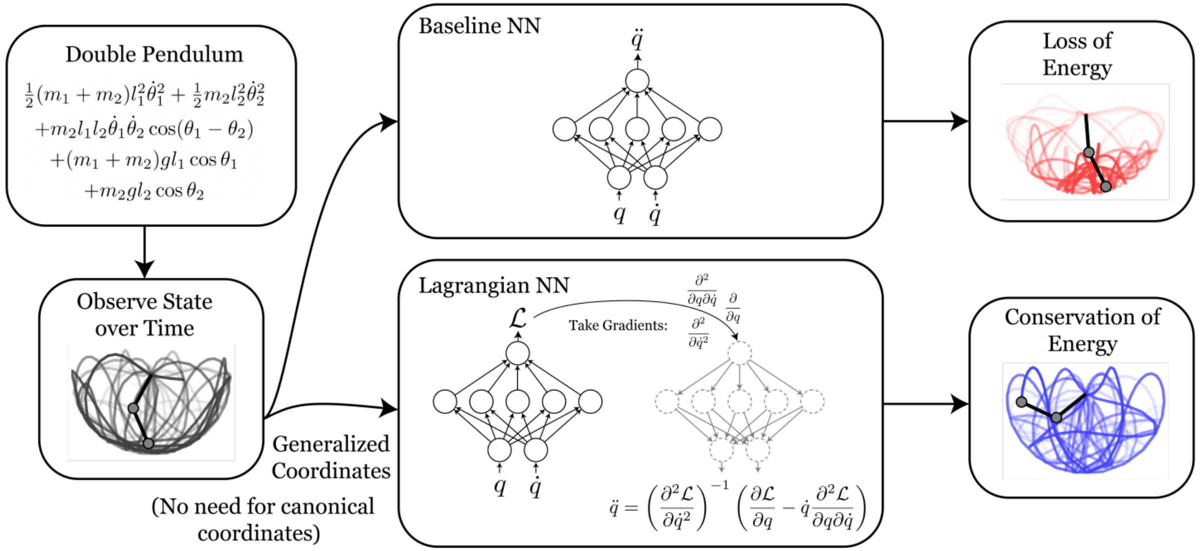
[8] Learning bifurcation diagram from single chaotic trajectory



Conservation Law

[10] Lagrangian neural network L

[Lagrangian Neural Network]

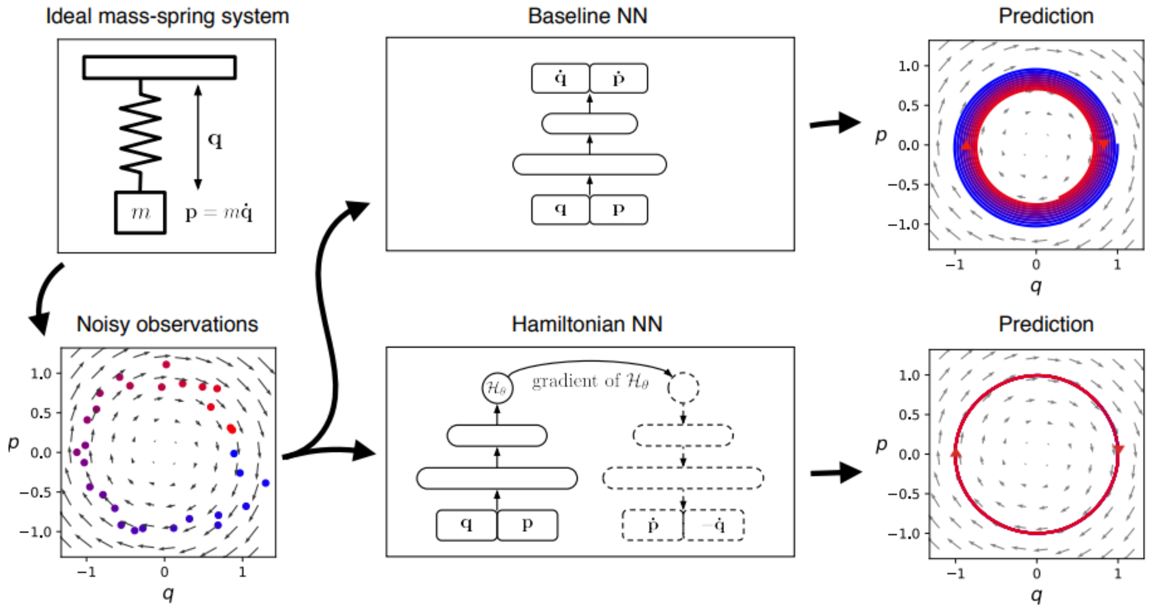


$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_j} = \frac{\partial \mathcal{L}}{\partial q_j}.$$

$$\boxed{\ddot{q} = (\nabla_{\dot{q}}\nabla_{\dot{q}}^{\top}\mathcal{L})^{-1}[\nabla_q \mathcal{L} - (\nabla_q \nabla_{\dot{q}}^{\top}\mathcal{L})\dot{q}].}$$

[11] Hamiltonian neural network H

[Hamiltonian Neural Network]



$$\frac{d\mathbf{q}}{dt} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}}, \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}}.$$

Discussion

- (1) Data representation
  - Video
    - Extract only physically relevant variables [1][12]
    - Disentangle physics and form factors [2][3]
  - Low-dim physical trajectory [4] → Good!
  - High-dim physical trajectory/fields
    - Collective coordinate: [5][16]
    - Quantization of particles/supercells: Perception + GNN [6][13][14]
    - Renormalizing flow [?Multi-scale models]

Global modes

Trade-Off?

Locality in space

Combination & Interplay

Learning effective Lagrangian/Hamiltonian

- (2) Learning goal
  - Equation
    - Sparse regression [5]
    - Recurrent neural models [1][2]
    - Symbolic regression
      - First numeric, then symbolic [6]
      - Numeric-symbolic hybrid system [15]
  - Pattern
    - Bifurcation diagram [7][8]
    - Conservation Law, Symmetry [10][11][12]
    - General conservation law (other than Hamiltonian or Lagrangian)?
    - Periodic orbit, regular-chaotic phase transition [9]