NTNU
Norwegian University of Science and Technology

SINDy – a survey of methods and their properties

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Trial lecture
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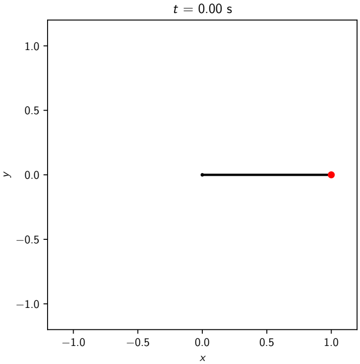
Data-driven discovery of dynamical systems



We want to find the differential equation $\dot{\boldsymbol{x}}(t) = X(\boldsymbol{x}(t))$, $X : \mathbb{R}^2 \to \mathbb{R}^2$, generating the trajectory in the movie.

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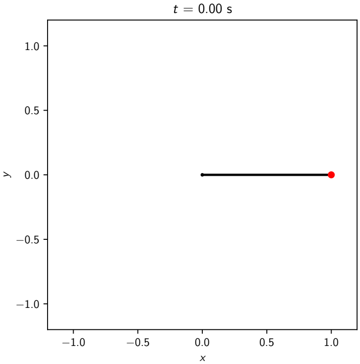

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Outline of the procedure

We define

$$\begin{cases} \dot{x} = \sum_{i=1}^{N_x} \lambda_i f_i(x, y) \\ \dot{y} = \sum_{j=1}^{N_y} \mu_j g_j(x, y), \end{cases} \tag{1}$$

for a set of functions $f_i, g_j : \mathbb{R}^2 \to \mathbb{R}$, and look for a *good* set of coefficients λ_i, μ_j making (1) an accurate approximation of $\dot{\boldsymbol{x}}(t) = X(\boldsymbol{x}(t))$.

Sparse Identification of Nonlinear Dynamics (SINDy)

Motivation behind SINDy

The right-hand side of most differential equations is made of the sum of a few functions, so the coefficients λ_i, μ_j in the linear combination should be, in large part, set to zero.

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Some examples:

- Simple pendulum: $\dot{x} = y$, $\dot{y} = -g/L \sin(x)$,
- Lorenz: $\dot{x} = \sigma(y - x)$, $\dot{y} = x(\rho - z) - y$, $\dot{z} = xy - \beta z$,
- Free rigid body:

$$\dot{\boldsymbol{x}} = \begin{bmatrix} 0 & x_3/I_3 & -x_2/I_2 \\ -x_3/I_3 & 0 & x_1/I_1 \\ x_2/I_2 & -x_1/I_1 & 0 \end{bmatrix} \boldsymbol{x}.$$

Sparse Identification of Nonlinear Dynamics (SINDy)

The algorithm to approximate $X : \mathbb{R}^d \to \mathbb{R}^d$

1. Build the data and derivative matrices

$$U = \begin{bmatrix} \boldsymbol{x}(t_1) & \cdots & \boldsymbol{x}(t_m) \end{bmatrix}^\top, \; U_p = \begin{bmatrix} \dot{\boldsymbol{x}}(t_1) & \cdots & \dot{\boldsymbol{x}}(t_m) \end{bmatrix}^\top \in \mathbb{R}^{m \times d}.$$

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2. Choose $f_1, \dots, f_N : \mathbb{R}^d \to \mathbb{R}$ that are likely to appear in X, and define the matrix $\Theta(U) \in \mathbb{R}^{m \times N}$ with entries

$$\Theta(U)_{i,j} = f_j(\boldsymbol{x}(t_i)), \; i = 1, \dots, m, \; j = 1, \dots, N.$$

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3. Solve

$$\min_{\Sigma\in\mathbb{R}^{N\times d}} \|U_p - \Theta(U)\Sigma\|_F^2 + \lambda \|\mathrm{vec}(\Sigma)\|_1 \,, \;\; \lambda > 0.$$

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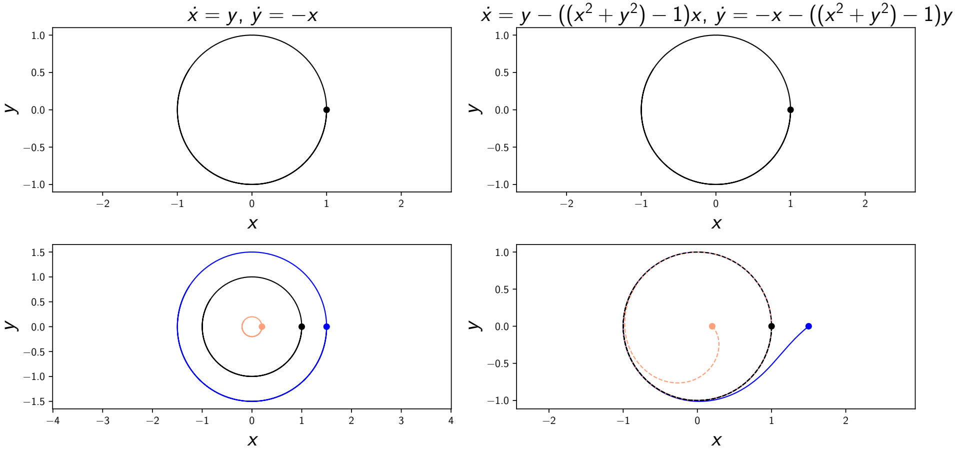
Building the data matrix



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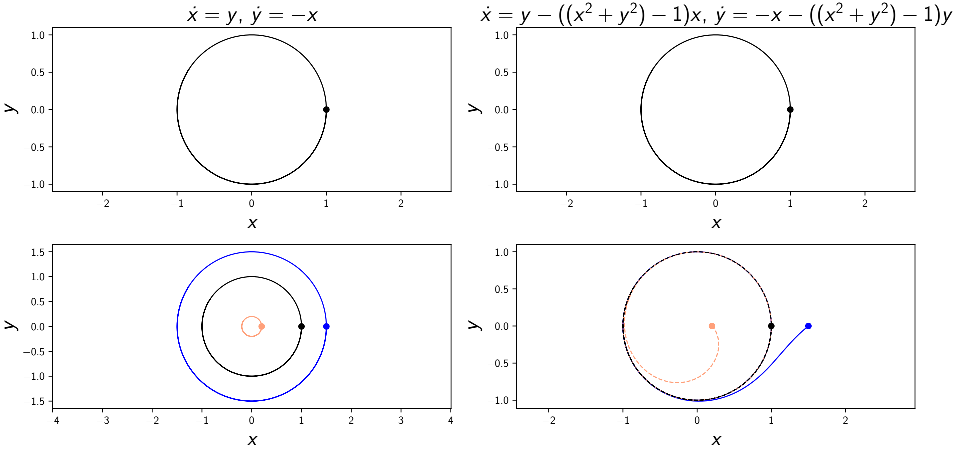

- The data matrix $U \in \mathbb{R}^{m \times d}$ collects the snapshots of some observed trajectories at different time instants $t_1, \dots, t_m$. Typically $d \ll m$.

Building the derivative matrix

- We generally do not know the exact values of $\dot{\boldsymbol{x}}(t_i)$, i.e., of $X(\boldsymbol{x}(t_i))$, so we need to approximate them to assemble $U_p \in \mathbb{R}^{m\times d}$.

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- Approximating the derivatives is a delicate step that could amplify the noise present in the trajectory data.

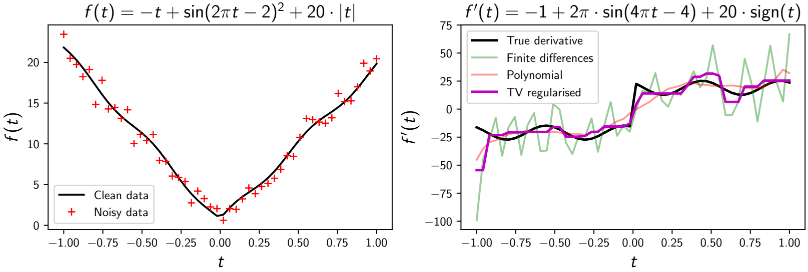

Figure: Results obtained with the PySINDy[1] library.

[1] Alan A Kaptanoglu et al. “PySINDy: A comprehensive Python package for robust sparse system identification”. In: *arXiv preprint arXiv:2111.08481* (2021).

Total Variation Regularised Derivative

- Let $[t_1, t_m] \ni t \mapsto x(t) \in \mathbb{R}$ be a signal with derivative $u(t)$.
- Consider a vector $\boldsymbol{s} \in \mathbb{R}^m$ made of noisy entries $s_i = x(t_i) + \delta_i$.

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- Consider a vector $\boldsymbol{s} \in \mathbb{R}^m$ made of noisy entries $s_i = x(t_i) + \delta_i$.
- The TV regularised derivative based on $\boldsymbol{s} \in \mathbb{R}^m$ is defined as

$$\operatorname*{arg\,min}_{\boldsymbol{u} \in \mathbb{R}^m} F(\boldsymbol{u}) := \frac{1}{2} \left\| A\boldsymbol{u} - (\boldsymbol{s} - s_1) \right\|_2^2 + \alpha \left\| D\boldsymbol{u} \right\|_1 .$$

  The matrix A contains quadrature weights, so

$$(A\boldsymbol{u})_i \approx \int_{t_1}^{t_i} u(t)\mathrm{d}t,$$

  while D is a finite differences matrix of the first order, so

$$(D\boldsymbol{u})_i \approx \dot{u}(t_i).$$

Building a library of candidate functions

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- For example, if we consider polynomials up to degree 2 for a system in $\mathbb{R}^2$, we would have

$$\Theta(U) = \begin{bmatrix} 1 & x(t_1) & y(t_1) & x(t_1)^2 & x(t_1)y(t_1) & y(t_1)^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x(t_m) & y(t_m) & x(t_m)^2 & x(t_m)y(t_m) & y(t_m)^2 \end{bmatrix} \in \mathbb{R}^{m\times 6}.$$

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- Another common set of functions are trigonometric functions, for example in the pendulum $\ddot{x} = -g/L\sin(x)$. Thus, one can augment the polynomial dictionary with functions like $\sin(kx)$, $k \in \mathbb{Z}$.

Least squares with sparsity promotion

- We now need to find how to linearly combine the columns of $\Theta(U)$ to recover U_p, with a sparse set of coefficients.

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- A first strategy to do so is ℓ^1 regularisation, leading to the (convex) unconstrained minimisation problem

$$\min_{\Sigma \in \mathbb{R}^{N \times d}} \|U_p - \Theta(U)\Sigma\|_F^2 + \lambda \|\mathrm{vec}(\Sigma)\|_1 , \quad \lambda > 0,$$

or, equivalently, to the inequality-constrained problem

$$\min_{\Sigma \in \mathbb{R}^{N \times d}} \|U_p - \Theta(U)\Sigma\|_F^2 , \quad \text{s.t.} \quad \|\mathrm{vec}(\Sigma)\|_1 < \mathrm{tol}.$$

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- This method can be expensive, especially for high-dimensional datasets.

The sequential thresholded least squares method

- The alternative approach recommended in the original paper[2] is the *Sequential Thresholded Least Squares method* (STLS).

[2] Steven L Brunton, Joshua L Proctor, and J Nathan Kutz. "Discovering governing equations from data by sparse identification of nonlinear dynamical systems". In: *Proceedings of the national academy of sciences* 113.15 (2016), pp. 3932–3937.

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2. For $k = 1, \ldots, K$ solve the constrained least squares problem

$$\Sigma^k := \operatorname*{arg\,min}_{\Sigma \in \mathbb{R}^{N \times d}} \| U_p - \Theta(U)\Sigma \|_F^2$$

$$\text{s.t. } \Sigma_{i,j} = 0 \text{ whenever } \Sigma_{i,j}^{k-1} < \lambda.$$

[2] Brunton, Proctor, and Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems".

STLS convergence properties[3]

$$F(\Sigma) = \left\| U_p - \Theta(U)\Sigma \right\|_F^2 + \lambda^2 \left\| \mathrm{vec}(\Sigma) \right\|_0 . \tag{2}$$

[3] Linan Zhang and Hayden Schaeffer. “On the convergence of the SINDy algorithm”. In: *Multiscale Modeling & Simulation* 17.3 (2019), pp. 948–972.

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Convergence theorem

Suppose that $\|\Theta(U)\|_2 = 1$.

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4. The iterates $\{\Sigma^k\}$ strictly decrease (2) unless stationary.

[3] Zhang and Schaeffer, "On the convergence of the SINDy algorithm".

Example: Simple harmonic oscillator

The target equations are

$$\begin{cases} \dot{x}(t) = y(t) \\ \dot{y}(t) = -0.5\,x(t). \end{cases}$$

Result obtained with **LASSO**, fixing $\lambda = 10^{-3}$ and exact derivatives $\dot{\boldsymbol{x}}(t_i)$:

$$\begin{array}{c} \\ 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{array} \begin{array}{c} \begin{array}{cc} \dot{x} & \dot{y} \end{array} \\ \begin{bmatrix} 0 & 0 \\ 0 & -0.4996 \\ 0.9991 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \end{array}.$$

Result obtained with **STLS**, fixing $\lambda = 0.05$ and exact derivatives $\dot{\boldsymbol{x}}(t_i)$:

$$\begin{array}{c} \\ 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{array} \begin{array}{c} \begin{array}{cc} \dot{x} & \dot{y} \end{array} \\ \begin{bmatrix} 0 & 0 \\ 0 & -0.5 \\ 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \end{array}.$$

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Example with noisy data

Target differential equations: $\begin{cases} \dot{x} = -0.1x + 2y \\ \dot{y} = -2x - 0.1y \end{cases}.$

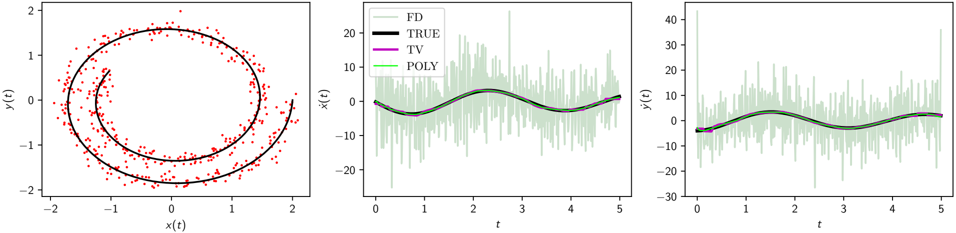

Figure: Gaussian noise with $\sigma = 0.1$. STLS algorithm with $\lambda = 0.05$.

POLY: $\begin{cases} \dot{x} = -0.082x + 1.975y \\ \dot{y} = -1.972x - 0.110y \end{cases}$, TV: $\begin{cases} \dot{x} = -0.092x + 1.974y \\ \dot{y} = -1.981x - 0.107y. \end{cases}$

Constraining the coefficients

- Suppose we know we are dealing with a planar Hamiltonian system of the form
$$\begin{cases} \dot{x} = y \\ \dot{y} = -V'(x), \end{cases} \tag{3}$$
where we do not know the potential energy $V : \mathbb{R} \to \mathbb{R}$.

- Then we could constrain the optimisation problem further, for example saying that there is no term in y in the second equation.

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- Then we could constrain the optimisation problem further, for example saying that there is no term in y in the second equation.
- The same might occur when we know part of the terms on the right-hand side, conservation laws, or symmetries in the equations.
- To see how to impose the structure in (3), we first rewrite the SINDy method in vector form.

Vector version of SINDy

- We use the vec operator, which stacks the columns of a matrix into a single column vector:

$$\operatorname{vec}\left(\begin{bmatrix} \boldsymbol{a}_1 & \boldsymbol{a}_2 & \cdots & \boldsymbol{a}_k \end{bmatrix}\right) = \begin{bmatrix} \boldsymbol{a}_1^\top & \cdots \boldsymbol{a}_k^\top \end{bmatrix}^\top .$$

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This operator also satisfies $\operatorname{vec}(ABC) = (C^\top \otimes A)\operatorname{vec}(B)$, and hence

$$\operatorname{vec}(\Theta(U)\Sigma) = (I_d \otimes \Theta(U))\operatorname{vec}(\Sigma) =: \widetilde{\Theta}(U)\boldsymbol{\sigma} \in \mathbb{R}^{m \cdot d}.$$

More explicitly, $\widetilde{\Theta}(U)$ is of the form

$$\widetilde{\Theta}(U) = \begin{bmatrix} \Theta(U) & 0 & \cdots & 0 \\ 0 & \Theta(U) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Theta(U) \end{bmatrix}.$$

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$$\mathrm{vec}(\Theta(U)\Sigma) = (I_d \otimes \Theta(U))\,\mathrm{vec}(\Sigma) =: \widetilde{\Theta}(U)\boldsymbol{\sigma} \in \mathbb{R}^{m \cdot d}.$$

- Since $\|A\|_F = \|\mathrm{vec}(A)\|_2$, the LASSO formulation can be rewritten as

$$\text{Find } \underset{\boldsymbol{\sigma} \in \mathbb{R}^{N \cdot d}}{\arg\min} \left\| \widetilde{\Theta}(U)\boldsymbol{\sigma} - \boldsymbol{u}_p \right\|_2^2 + \lambda \left\| \boldsymbol{\sigma} \right\|_1 ,$$

where $\boldsymbol{u}_p := \mathrm{vec}(U_p)$.

The constrained STLS algorithm[4]

- With the vector notation, one of the STLS iterates is of the form

$$\boldsymbol{\sigma}^k := \underset{\boldsymbol{\sigma} \in \mathbb{R}^{N \cdot d}}{\arg\min} \left\| \widetilde{\Theta}(U)\boldsymbol{\sigma} - \boldsymbol{u}_p \right\|_2^2$$
$$\text{s.t. } C^k \boldsymbol{\sigma} = \boldsymbol{d}^k, \quad C^k \in \mathbb{R}^{r_k \times N \cdot d},$$

which admits a unique solution if

$$\mathrm{rank}(C^k) = r_k, \text{ and } \mathrm{rank}\left(\begin{bmatrix} \widetilde{\Theta}(U) \\ C^k \end{bmatrix} \right) = N \cdot d.$$

[4] Jean-Christophe Loiseau and Steven L Brunton. "Constrained sparse Galerkin regression". In: *Journal of Fluid Mechanics* 838 (2018), pp. 42–67.

Back to planar Hamiltonian systems...

- Say that we want to discover $\ddot{x} = -V'(x)$ with $V(x) = x^2/4$. We can then include prior information as $\widetilde{C}\boldsymbol{\sigma} = \widetilde{\boldsymbol{d}}$ where

$$\widetilde{C} = \begin{array}{c} \begin{array}{cc} \dot{x} \qquad\qquad & \dot{y} \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \\ \begin{array}{cccccc} 1 & x & y & 1 & x & y \end{array} \end{array}, \quad \widetilde{\boldsymbol{d}} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

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- At each step, we can then solve

$$\boldsymbol{\sigma}^k := \underset{\boldsymbol{\sigma} \in \mathbb{R}^{N \cdot d}}{\arg\min} \left\| \widetilde{\Theta}(U)\boldsymbol{\sigma} - \boldsymbol{u}_p \right\|_2^2$$

$$\text{s.t. } \begin{bmatrix} C^k \\ \widetilde{C} \end{bmatrix} \boldsymbol{\sigma} = \begin{bmatrix} \boldsymbol{d}^k \\ \widetilde{\boldsymbol{d}} \end{bmatrix}.$$

Constraining the model in the presence of noise

We now perturb the exact derivatives $\dot{\boldsymbol{x}}(t_i)$ to $\boldsymbol{v}_i = \dot{\boldsymbol{x}}(t_i) + \varepsilon$ with $\varepsilon_k \sim \mathcal{N}(0, \sigma^2)$, $k = 1, \ldots, d$, and see how the reconstructed models are.

The target equations are $\dot{x} = y$, $\dot{y} = -0.5x$.

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The orange matrices are obtained with constrained models, while the blue ones are unconstrained:

$$
\begin{array}{cc}
 & \sigma = 10^{-3} \\
\begin{array}{c} 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{array} & \begin{bmatrix} 0 & 0 \\ 0 & -0.500 \\ 1.000 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} \\
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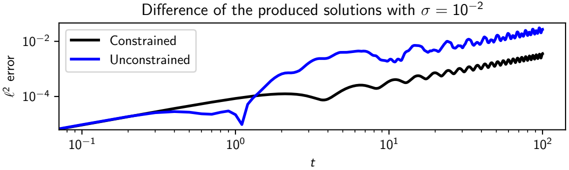
\begin{array}{c}
\sigma = 10^{-2} \\
\begin{bmatrix} 0 & 0.112 \\ 0 & -0.500 \\ 1.000 & 0 \\ 0 & -0.112 \\ 0 & 0 \\ 0 & -0.223 \end{bmatrix} \\
\begin{array}{cc} \dot{x} & \dot{y} \end{array}
\end{array}.
$$

Analysis of the recovered dynamics

$$\Sigma = \begin{array}{c} \left[\begin{array}{cc} 0 & 0.112 \\ 0 & -0.500 \\ 1.000 & 0 \\ 0 & -0.112 \\ 0 & 0 \\ 0 & -0.223 \end{array}\right] \end{array}\begin{array}{l} 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{array} \implies \begin{cases} \dot{x} = y \\ \dot{y} = -0.5x + c(1 - x^2 - 2y^2), \; c \approx 0.112. \end{cases}$$

The additional term vanishes on the energy level set of the initial condition $\boldsymbol{x}_0 = [1, 0]$, which is the ellipse

$$\left\{(x, y) \in \mathbb{R}^2 : \; H(x, y) = y^2/2 + x^2/4 = 1/4\right\}.$$



SINDy for discrete dynamical systems

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$$U_l = \begin{bmatrix} \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_m \end{bmatrix}^\top, \; U_r = \begin{bmatrix} \boldsymbol{x}_2 & \cdots & \boldsymbol{x}_{m+1} \end{bmatrix}^\top \in \mathbb{R}^{m\times d}.$$

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- We can still apply the same procedure as SINDy for continuous systems, but to these new data matrices:

$$\min_{\Sigma \in \mathbb{R}^{N \times d}} \|U_r - \Theta(U_l)\Sigma\|_F^2 + \lambda \|\mathrm{vec}(\Sigma)\|_1, \; \lambda > 0.$$

SINDy for parametric differential equations

- What we have seen up to now extends to dynamical systems that depend on a parameter $\boldsymbol{\mu} \in \mathbb{R}^p$.
- We can rewrite
$$\dot{\boldsymbol{x}} = X(\boldsymbol{x}, \boldsymbol{\mu})$$
as
$$\begin{cases} \dot{\boldsymbol{x}} = X(\boldsymbol{x}, \boldsymbol{\mu}) \\ \dot{\boldsymbol{\mu}} = 0. \end{cases} \tag{4}$$
- SINDy can then be applied to (4) using the new state variable
$$\boldsymbol{z} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{\mu} \end{bmatrix}.$$

SINDy for non-autonomous differential equations

- A similar reasoning applies to explicitly time-dependent differential equations.
- We can rewrite
$$\dot{\boldsymbol{x}} = X(\boldsymbol{x}, t)$$
as
$$\begin{cases} \dot{\boldsymbol{x}} = X(\boldsymbol{x}, t) \\ \dot{t} = 1. \end{cases} \tag{5}$$
- SINDy can then be applied to (5) using the new state variable
$$\boldsymbol{z} = \begin{bmatrix} \boldsymbol{x} \\ t \end{bmatrix}.$$

Some limitations and extensions of SINDy

Curse of dimensionality[5]

As the dimension d grows, the set of basis functions one has to consider will grow quickly. For example $\dim(\mathbb{P}_k^d) = \binom{k+d}{d}$, which for $d = 6$ and $k = 5$ is already 462.

[5] Kathleen Champion et al. "Data-driven discovery of coordinates and governing equations". In: *Proceedings of the National Academy of Sciences* 116.45 (2019), pp. 22445–22451; Brunton, Proctor, and Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems".

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A common solution to this problem is to start with a truncated SVD:

$$U^\top \approx \Psi_r \Sigma_r V_r^\top \implies \boldsymbol{x} \approx \Psi_r \boldsymbol{a}, \quad \boldsymbol{a} \in \mathbb{R}^r.$$

Then, one can apply the SINDy algorithm in the variable $\boldsymbol{a}$, and $\dot{\boldsymbol{x}}(t) \approx \Psi_r \dot{\boldsymbol{a}}(t)$.

[5] Champion et al., "Data-driven discovery of coordinates and governing equations"; Brunton, Proctor, and Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems".

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Knowledge of the terms to include in the dictionary

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A solution[6] could be to use general enough parametric models like Neural ODEs

$$\dot{\boldsymbol{x}}(t) = \mathcal{N}_{\theta}(\boldsymbol{x}(t)), \;\; \theta \in \mathbb{R}^{p},$$

to get a first approximation of the right-hand side. We could then do sparse regression over this approximate model to get a more interpretable approximation, as in SINDy.

[6] Christopher Rackauckas et al. “Universal differential equations for scientific machine learning”. In: *arXiv preprint arXiv:2001.04385* (2020).

Approximating the derivatives

The SINDy algorithm depends on having an accurate approximation of the exact derivative matrix U_p.

[7] Hayden Schaeffer and Scott G McCalla. "Sparse model selection via integral terms". In: *Physical Review E* 96.2 (2017), p. 023302.

Approximating the derivatives

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A solution[7] can be to work with the integral version of the differential equation:

$$\boldsymbol{x}(t) - \boldsymbol{x}(0) = \int_0^t X(\boldsymbol{x}(t))\mathrm{d}t.$$

We can then proceed similarly to the SINDy algorithm and write

$$x_i(t_m) - x_i(0) \approx \sum_{j=1}^{N} \Sigma_{i,j} d_j(t_m), \quad d_j(t_m) \approx \int_0^{t_m} f_j(\boldsymbol{x}(t))\mathrm{d}t.$$

[7]Schaeffer and McCalla, "Sparse model selection via integral terms".

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THANK YOU FOR THE ATTENTION

Example in higher dimensions

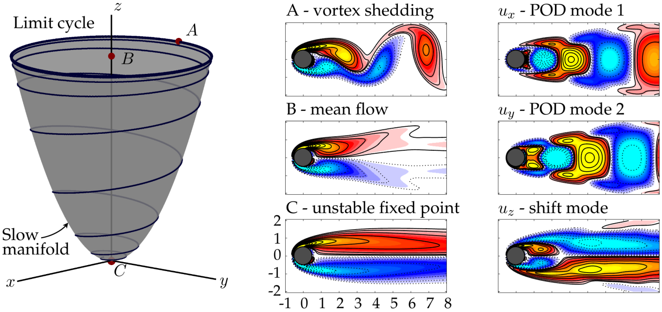
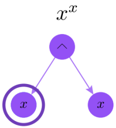


Figure: Low-rank dynamics underlying the periodic vortex shedding behind a circular cylinder at low Reynolds number, $Re = 100$.

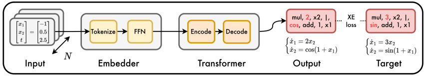
$$\begin{cases} \dot{x} = \mu x - \omega y + Axz \\ \dot{y} = \omega x + \mu y + Ayz \\ \dot{z} = -\lambda(z - x^2 - y^2). \end{cases}$$

Some alternative methods to SINDy

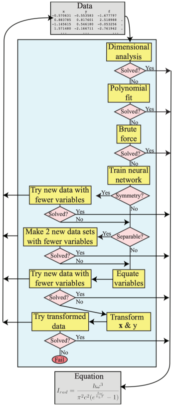
- Symbolic regression with evolutionary algorithms[1].



- Symbolic regression with transformers[2]



- Hybrid approaches, like AI Feynman[3]



[1] Miles Cranmer. “Interpretable machine learning for science with PySR and SymbolicRegression. jl”.

[2] Stéphane d’Ascoli et al. “Odeformer: Symbolic regression of dynamical systems with transformers”.

[3] Silviu-Marian Udrescu and Max Tegmark. “AI Feynman: A physics-inspired method for symbolic regression”.

PDE-FIND[1]

- Similarly to SINDy, we could discover the right-hand side of the PDE

$$\partial_t u(\boldsymbol{x}, t) = \mathcal{N}\left(u, \partial_x u, \partial_{xx} u, \dots\right), \quad \boldsymbol{x} \in \mathbb{R}^d.$$

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- This time, the dataset is a vector $\boldsymbol{u} \in \mathbb{R}^{M \cdot N}$ where

$$\boldsymbol{u} = \mathrm{vec}(U), \;\; U_{n,m} \approx u(\boldsymbol{x}_n, t_m), \;\; n = 1, \ldots, N, \;\; m = 1, \ldots, M,$$

for a spatio-temporal grid $\{(\boldsymbol{x}_n, t_m)\}$ of $\Omega \times [0, T]$, $\Omega \subset \mathbb{R}^d$.

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  for a spatio-temporal grid $\{(\boldsymbol{x}_n, t_m)\}$ of $\Omega \times [0, T]$, $\Omega \subset \mathbb{R}^d$.
- The candidate matrix becomes

$$\Theta(U) = \begin{bmatrix} 1 & \boldsymbol{u} & \boldsymbol{u}_x & \boldsymbol{u} \odot \boldsymbol{u}_x & \cdots \end{bmatrix} \in \mathbb{R}^{N \cdot M \times K}$$

  and we have to deal with a sparse regression of the form

$$\min_{\boldsymbol{\sigma} \in \mathbb{R}^K} \|\boldsymbol{u}_t - \Theta(U)\boldsymbol{\sigma}\|_2^2 + \lambda R(\boldsymbol{\sigma}).$$

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