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Discovering governing equations from data by sparse identification of nonlinear dynamical systems

Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz Authors Info & Affiliations

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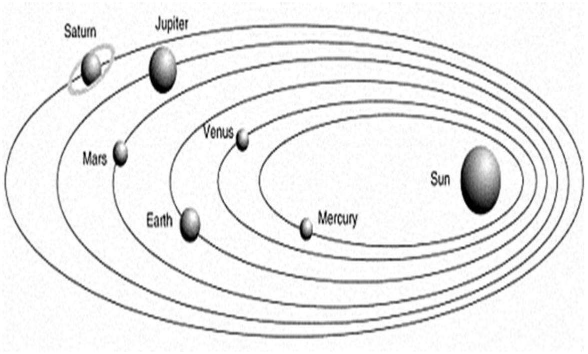
An analogy!

Kepler developed a data-driven model for planetary motion, resulting in his famous elliptic orbits. However, this model did not explain the fundamental dynamic relationships that give rise to planetary orbits, or provide a model for how these bodies react when perturbed.

Newton, in contrast, discovered a dynamic relationship between momentum and energy that described the underlying processes responsible for these elliptic orbits. This dynamic model may be generalized to predict behavior in regimes where no data were collected.

Kepler's Elliptical Orbits



$$F = G\frac{m_1 m_2}{r^2}$$

Main Message

- Extracting governing equations from data is important
- Understanding patterns in vast multimodal data that are beyond the ability of humans to grasp!
- Governing equations can be discovered even from noisy measurement data.
- Our assumption about the structure of the model is that there are only a few important terms that govern the dynamics, so that the equations are sparse in the space of possible functions; this assumption holds for many physical systems in an appropriate basis.

Sparse Identification of Nonlinear Dynamics (SINDy)

Here, we consider dynamical systems (31) of the form

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t)). \quad \textbf{[1]}$$

The vector $\mathbf{x}(t) \in \mathbb{R}^n$ denotes the state of a system at time t, and the function $\mathbf{f}(\mathbf{x}(t))$ represents the dynamic constraints that define the equations of motion of the system, such as Newton's second law. Later, the dynamics will be generalized to include parameterization, time dependence, and forcing.

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}^T(t_1) \\ \mathbf{x}^T(t_2) \\ \vdots \\ \mathbf{x}^T(t_m) \end{bmatrix} = \overbrace{\begin{bmatrix} x_1(t_1) & x_2(t_1) & \cdots & x_n(t_1) \\ x_1(t_2) & x_2(t_2) & \cdots & x_n(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ x_1(t_m) & x_2(t_m) & \cdots & x_n(t_m) \end{bmatrix}}^{\text{state}\ \longrightarrow} \downarrow \text{time}$$

$$\dot{\mathbf{X}} = \begin{bmatrix} \dot{\mathbf{x}}^T(t_1) \\ \dot{\mathbf{x}}^T(t_2) \\ \vdots \\ \dot{\mathbf{x}}^T(t_m) \end{bmatrix} = \begin{bmatrix} \dot{x}_1(t_1) & \dot{x}_2(t_1) & \cdots & \dot{x}_n(t_1) \\ \dot{x}_1(t_2) & \dot{x}_2(t_2) & \cdots & \dot{x}_n(t_2) \\ \vdots & \vdots & \ddots & \vdots \\ \dot{x}_1(t_m) & \dot{x}_2(t_m) & \cdots & \dot{x}_n(t_m) \end{bmatrix}.$$

Sparse Identification of Nonlinear Dynamics (SINDy)

Next, we construct a library $\Theta(\mathbf{X})$ consisting of candidate nonlinear functions of the columns of $\mathbf{X}$. For example, $\Theta(\mathbf{X})$ may consist of constant, polynomial, and trigonometric terms:

$$\Theta(\mathbf{X}) = \begin{bmatrix} | & | & | & | & & | & | & \\ 1 & \mathbf{X} & \mathbf{X}^{P_2} & \mathbf{X}^{P_3} & \cdots & \sin(\mathbf{X}) & \cos(\mathbf{X}) & \cdots \\ | & | & | & | & & | & | & \end{bmatrix}. \quad \textbf{[2]}$$

Each column of $\Theta(\mathbf{X})$ represents a candidate function for the right-hand side of Eq. **1**. There is tremendous freedom in choosing the entries in this matrix of nonlinearities. Because we believe that only a few of these nonlinearities are active in each row of $\mathbf{f}$, we may set up a sparse regression problem to determine the sparse vectors of coefficients $\Xi = [\boldsymbol{\xi}_1\ \boldsymbol{\xi}_2\ \cdots\ \boldsymbol{\xi}_n]$ that determine which nonlinearities are active:

$$\dot{\mathbf{X}} = \Theta(\mathbf{X})\Xi. \quad \textbf{[3]}$$

Derivative of X with time

A matrix of candidate functions

Unknown,
a matrix of sparse vectors of coefficients

example: Chaotic Lorenz System

Lorenz system is a set of ordinary differential equations is notable for having chaotic solutions for certain parameter values and initial conditions. In particular, the Lorenz attractor is a set of chaotic solutions of the Lorenz system.

equations:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \sigma(y - x),$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = x(\rho - z) - y,$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = xy - \beta z.$$

A sample solution in the Lorenz attractor when:
$\rho = 28$, $\sigma = 10$, and $\beta = 8/3$

example: Chaotic Lorenz System

The unknown matrix of weights can be computed by solving the Linear system of equation.

Resulting matrix wont be as clear as this example, but by eleminating functions with trivial weights the matrix becomes sparse.

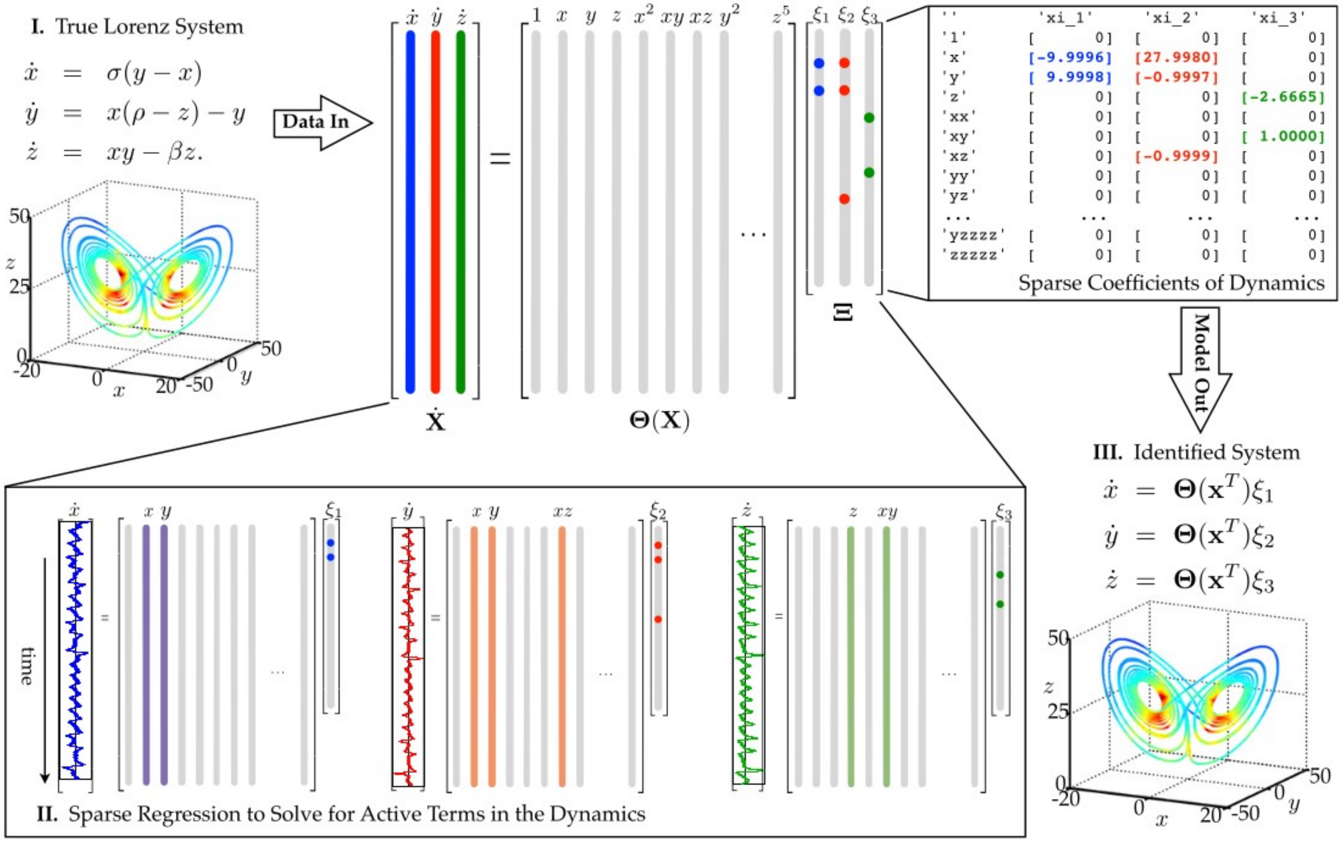


Fig. 1. Schematic of the SINDy algorithm, demonstrated on the Lorenz equations. Data are collected from the system, including a time history of the states $\mathbf{X}$ and derivatives $\dot{\mathbf{X}}$; the assumption of having $\dot{\mathbf{X}}$ is relaxed later. Next, a library of nonlinear functions of the states, $\Theta(\mathbf{X})$, is constructed. This nonlinear feature library is used to find the fewest terms needed to satisfy $\dot{\mathbf{X}} = \Theta(\mathbf{X})\Xi$. The few entries in the vectors of Ξ, solved for by sparse regression, denote the relevant terms in the right-hand side of the dynamics. Parameter values are $\sigma = 10, \beta = 8/3, \rho = 28$, $(x_0, y_0, z_0)^T = (-8, 7, 27)^T$. The trajectory on the Lorenz attractor is colored by the adaptive time step required, with red indicating a smaller time step.

Discussion

- It was assumed that a few important terms that govern the dynamics, and there are no other differential terms inside equations.
- Open question, how to know if differential terms are present in the governing dynamics of a dataset?