Learning nonlinear dynamics using linear regression

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PRINCETON UNIVERSITY
Data-driven modeling

We will consider discrete-time dynamical systems, either linear:

\[ x_{t+1} = Ax_t \]

or nonlinear:

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- We wish to learn the matrix \( A \) or the function \( f \) directly from data.
- The data could be samples of the full state \( x_t \), or it could be some function \( \psi(x_t) \).
- We are also interested in control (i.e., \( x_{t+1} = Ax_t + Bu_t \) or \( f(x_t, u_t) \)), but here we will focus on the case without an input \( u \).
Suppose the system is linear:

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with \( x_t \in \mathbb{R}^n \). Suppose we observe \( x_1, x_2, \ldots, x_m \).
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- If \( m > n \), the problem is easy: we can just solve for \( A \).
- If \( m < n \), could find a minimum-norm \( A \) that fits the data.
- If data is noisy, there might not be an \( A \) that perfectly fits the data, but could find a least-squares solution (regression).
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Reduced-order models

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- Suppose the state dimension is very large (\( n \gg m \)), and we don’t want to actually compute the whole matrix \( A \). Can we compute, say, the dominant eigenvectors of \( A \)?
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- Suppose the state dimension is very large (\( n \gg m \)), and we don’t want to actually compute the whole matrix \( A \). Can we compute, say, the dominant eigenvectors of \( A \)?
- These would be useful in developing a reduced-order model for the dynamics: model only the behavior of the dominant eigenvectors, not the whole state.
Dynamic mode decomposition

- Dynamic Mode Decomposition\(^1\) approximates these eigenvectors ("DMD modes") using an Arnoldi-like algorithm:

\[
\begin{align*}
\text{Consider the subspace spanned by } & \{x_1, Ax_1, A^2x_1, \ldots, A^{m-1}x_1\} \\
\text{Act on this subspace by } & A \\
\text{and project back onto the subspace. Call this operator } & \hat{A} \\
\text{"DMD modes" are eigenvectors of } & \hat{A} \\
\end{align*}
\]

This method is also related to regression\(^2\): these eigenvectors ("DMD modes") are (projections of) eigenvectors of the matrix \(\hat{A}\) that is the least-squares solution to

\[
\begin{bmatrix} x_2 \cdots x_m \end{bmatrix} = \hat{A} \begin{bmatrix} x_1 \cdots x_{m-1} \end{bmatrix}
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Now consider a nonlinear system

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where we again observe \( x_1, x_2, \ldots, x_m. \)
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Try to find a function \( f(x) \) that fits the data.
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One approach

Try to find a function \( f(x) \) that fits the data.

- Specify some basis functions \( \varphi_j(x), j = 1, \ldots, N. \)
- Suppose

\[ f(x) = \sum_{j=1}^{N} c_j \varphi_j(x). \]

- Solve for the constants \( c_j \) that best fit the data.
Some difficulties

- We want to have a large set of basis functions ($N$ large), so that we can represent lots of different functions $f$. 
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- We want to have a large set of basis functions ($N$ large), so that we can represent lots of different functions $f$.
- However, if we make $N$ too large (compared to the available data), we will overfit the data.
For instance, consider fitting the 11 data points shown with a polynomial of degree 10:
Overfitting

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The curve perfectly interpolates the data, but does not represent the observed behavior.
Overfitting

A “better” fit is obtained by a polynomial of lower degree (here, degree 7) that does not perfectly interpolate the data:
Dealing with overfitting

There are some ways of avoiding overfitting.

\[ f(x) = \sum_{j=1}^{N} c_j \phi_j(x) \]

▶ Require that the vector \((c_1, \ldots, c_N)\) be sparse (only a few nonzero components)
▶ Add a penalty to encourage this: e.g.,
\[
\min c_j \left[ \| f(x) - \sum_{j=1}^{N} c_j \phi_j(x) \|_2^2 + \alpha \| c \|_1 \right].
\]

For more on this, see Rachel’s talk, and poster by Sam Otto.
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Nonlinear systems

Back to the nonlinear system

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Another approach

Try to find a change of coordinates \( z = h(x) \) such that the equations are particularly simple.
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Another approach

Try to find a change of coordinates \( z = h(x) \) such that the equations are particularly simple.

- Maybe even linear.
- Maybe even diagonal.
Example: two-dimensional map

Consider the map

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \begin{bmatrix} \lambda x_1 \\ \mu x_2 + (\lambda^2 - \mu) x_1^2 \end{bmatrix}.$$ 

This system has an equilibrium at the origin, and invariant manifolds given by $x_1 = 0$ and $x_2 = x_1^2$: 

![Diagram](attachment:image.png)
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Consider new coordinates

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\begin{align*}
  z_1 &= x_1 \\
  z_2 &= x_2 - x_1^2.
\end{align*}
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This system has an equilibrium at the origin, and invariant manifolds given by \(x_1 = 0\) and \(x_2 = x_1^2\):

Consider new coordinates \(z_1 = x_1\) and \(z_2 = x_2 - x_1^2\).

In the new coordinates, the dynamics become

\[
\begin{bmatrix}
    z_1 \\
    z_2
\end{bmatrix} \mapsto \begin{bmatrix}
    \lambda z_1 \\
    \mu z_2
\end{bmatrix}.
\]

Linear and diagonal (decoupled).
Why?

Why would we want to do this?

- Linear systems are easier to work with than nonlinear systems.
- Even if we have a model for a nonlinear system, control of such a system can be difficult.
- If we can find a mapping to a linear system, control is much easier: we have all the tools of linear control theory available.
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Even if we have a model for a nonlinear system
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  \[ x_{t+1} = f(x_t, u_t) \], control of such a system can be difficult.
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Is there a general way of obtaining such a change of coordinates?
To this end, consider a linear operator $U$ that acts on functions of the state $x$ as follows: for a function $g$, define

$$(Ug)(x) = g(f(x)),$$

where as before, $f$ describes the dynamics ($x_{t+1} = f(x_t)$).

- $U$ is a linear operator: $U(ag_1 + bg_2) = a(Ug_1) + b(Ug_2)$. 

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- Define a new coordinate $z = \varphi(x)$.
- Then $z$ evolves linearly:

$$z_{t+1} = \varphi(x_{t+1}) = \varphi(f(x_t)) = (U\varphi)(x_t) = \lambda \varphi(x_t) = \lambda z_t.$$
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$\blacktriangleright$ **$U$ is a linear operator:** $U(ag_1 + bg_2) = a(Ug_1) + b(Ug_2)$.

$\blacktriangleright$ **Suppose** $U$ **has an eigenfunction:** $U\varphi(x) = \lambda \varphi(x)$

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$\blacktriangleright$ **So if** $U$ **has eigenfunctions, and if we can find them, we know coordinates in which the dynamics are linear and diagonal.**
An extension of Dynamic Mode Decomposition can be used to find these eigenfunctions:

- Fix basis functions $\psi_1, \ldots, \psi_N$, functions of the state $x$.

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Extended Dynamic Mode Decomposition

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- Fix basis functions \( \psi_1, \ldots, \psi_N \), functions of the state \( x \).
- Gather data \( x_1, x_2, \ldots, x_m \).
- Find the matrix \( A \) that best fits

\[
\begin{bmatrix}
\psi_1(x_2) & \cdots & \psi_1(x_m) \\
\vdots & & \vdots \\
\psi_N(x_2) & \cdots & \psi_N(x_m)
\end{bmatrix}
= A
\begin{bmatrix}
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If \( U \) has an eigenfunction that lies in the span of \( \{ \psi_j \} \), then its eigenvalue is also an eigenvalue of \( A \), and the eigenfunction can be determined from the corresponding eigenvector of \( A \).

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Example: basins of attraction in the Duffing equation

Consider the Duffing equation

\[ \ddot{x} + \delta \dot{x} + x(x^2 - 1) = 0 \]

- Use extended DMD to find eigenfunctions of \( U \) (with \( \delta = 0.5 \)):
  - Data: \( 10^3 \) trajectories with 11 samples each, sampling interval \( \Delta t = 0.25 \)
  - Basis functions: 1000 radial basis functions (thin plate splines)
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  - Data: $10^3$ trajectories with 11 samples each, sampling interval $\Delta t = 0.25$
  - Basis functions: 1000 radial basis functions (thin plate splines)
  - $\lambda_0 = -10^{-14}$: corresponding eigenfunction is the constant function
  - $\lambda_1 = -10^{-3}$: eigenfunction reveals basins of attraction

![Diagrams showing basins of attraction]
Dynamics in each basin

\[ \lambda_2 = -0.237 + 1.387i \text{ (analytically } -0.250 + 1.392i) \]
What have we done?

- We have found coordinates in which the nonlinear system is linear and diagonal (decoupled).
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Caveats

- This required a lot of data: trajectories sampled throughout the state space (1000 trajectories of 11 samples each).
- One needs to specify a good choice of basis functions \( \{ \psi_j \} \).
- Fiddling is needed to avoid overfitting.
- Scales poorly for high-dimensional systems.
- Chaotic systems (specifically, “weak mixing” systems) do not have eigenfunctions!
Hao Zhang

- Online DMD algorithm: learn $x_{t+1} = Ax_t$ efficiently “on the fly”, as new data becomes available
  - rank-one updates to matrix $A$
  - gradually forget older data using a discount factor
  - Funded by AFOSR (Doug Smith, Gregg Abate)

Sam Otto

- Sparse system identification on the fly: perform nonlinear regression with a sparsity-promoting penalty, using an efficient algorithm that can be used in real time
Conclusions

- Regression methods can be used for linear and nonlinear systems
- For nonlinear systems, the choice of basis functions is critical
- Two perspectives:
  - Fit an ODE to data ($\dot{x} = Ax$ or $\dot{x} = f(x)$)
  - Find a change of coordinates in which the dynamics are linear and diagonal
- The former seems to be more promising for modeling on the fly