Inferring Untrained Dynamics of Complex Systems using Adapted Recurrent Neural Networks

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Dynamics Days Europe 2022
25 August 2022
• IFISC: Institute for Cross-Disciplinary Physics and Complex Systems in Mallorca.

• Joint research Institute of the University of the Balearic Islands (UIB) and the Spanish National Research Council (CSIC) created in 2007.
Complex Dynamics @ IFISC

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Feed forward Neural Network can approximate any continuous function (≥1 hidden layers + non-linear activations)

Recurrent Neural Networks can approximate dynamical systems

Video activity recognition

Running
• **Neuro-inspired concept**
  – Consider a “black-box (reservoir)“ complex recurrent network
  – The input nodes connected randomly to reservoir nodes
  – Output weights are trained

• **Generate nonlinear transient responses** to input

• **Mapping to a high-dimensional space**

Can emulate chaotic dynamical systems!
Lorenz model
\[
\begin{align*}
\dot{x} &= 10(y-x), \\
\dot{y} &= x(28-z) - y, \\
\dot{z} &= xy - 8z/3.
\end{align*}
\]

R → Echo State Network (popular variant of RC)

<table>
<thead>
<tr>
<th>Actual Lorenz system</th>
<th>R1 system</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Lambda_1$</td>
<td>0.91</td>
</tr>
<tr>
<td>$\Lambda_2$</td>
<td>0.00</td>
</tr>
<tr>
<td>$\Lambda_3$</td>
<td>-14.6</td>
</tr>
</tbody>
</table>

Infer unseen/untrained dynamics of systems by learning from a single example?

- physical models are parametrized → changing parameter leads to new behavior/dynamics
  \[ \dot{x}(t) = F(x(t), c) \]

- ML: statistical learning without being aware of parametrization of the physical model

- **Physics-informed machine learning**
  - Using physical knowledge to constrain the learning
  - biases on:
    - training data
    - loss function
    - network topology

Delay Systems

\[ \dot{x}(t) = F(x(t), x(t - \tau); p) \]

- Delays appear where signal propagation is finite
  - Neuroscience, photonics, epidemiologic models and control problems

- Rely on a continuous history function
  - Infinite dimensional

- For long delays these systems can become chaotic

\[ \lambda_{\text{max}} > 0 \]

Mackey-Glass system

SL with feedback
**Time lag** can be substantial in physiological systems

Example: following a loss of **blood cells**, it can take many days before new blood cells can be produced (activation, differentiation, and proliferation of the blood stem cells)

\[
\frac{dx}{dt} = \beta \frac{x_\tau}{1 + x_\tau^n} - \gamma x, \quad \gamma, \beta, n > 0,
\]

Mackey-Glass equation (for the **nonlinear production control** function)

- \(x\): concentration (assumed non-negative for all times) of circulating blood cells
- \(\beta, \gamma\) and \(n\): constants controlling the production of these cells
- \(x_\tau, x(t-\tau)\)

For some intermediate values of \(x_\tau\) the production rate would be adequate

If \(0 < x_\tau \ll 1\) individual would be sick and unable to generate enough blood cells

If \(1 \ll x_\tau\) person would have too many blood cells so that the production rate would once again be low

\[\beta=0.2, \gamma=0.1\text{ and }n=10\]

Mackey-Glass dynamics

\[ \frac{dx}{dt} = \beta \frac{x_{t}}{1 + x_{t}^{n}} - \gamma x, \]

\( \beta = 0.2, \gamma = 0.1 \) and \( n = 10 \)
Mackey-Glass dynamics

\[ \frac{dx}{dt} = \beta \frac{x_{\tau}}{1 + x_{\tau}^n} - \gamma x, \]

\( \beta = 0.2, \gamma = 0.1 \) and \( n = 10 \)

Possible to emulate with ML?
Delayed Echo State Networks

Incorporate a delay into the neural network

$$\tilde{x}(n+1) = \alpha \tilde{x}(n) + \beta \tanh(W \tilde{x}(n-D) + \gamma W_{in}s(n) + W_b)$$

Optimal prediction performance for data of Mackey Glass system ($\tau$) at $D=\tau$

- Optimizing hyperparameters with bayesian optimization
- Closed-loop mode: training the output layer and feeding back prediction

$$\tilde{x}(n+1) = \alpha \tilde{x}(n) + \beta \tanh(W \tilde{x}(n-D) + \gamma W_{in}W_{out}x(n) + W_b)$$

After training reconfigure network by setting delay $D$ to untrained values
→ Inferring unseen dynamical regimes
• Training for a long delay $D, \tau = 100$
• After training scanning $D$
• Learning one size enables to infer the entire bifurcation diagram

Possible to emulate with ML!
• Training at a delay of D=100
  † After training: reducing the delay length to D=30
  † Inference reveals unseen/untrained chaotic attractor
  † Lyapunov exponent can be precisely derived from the reservoir
• Method even reveals multistabilities of the Mackey-Glass system
Autocorrelation function (ACF)

\[ r_\tau = \frac{c_\tau}{c_0}, \quad c_\tau = \frac{1}{N} \sum_{t=1}^{N-\tau} (x_t - \langle X \rangle)(x_{t+\tau} - \langle X \rangle) \]

- Adapted Echo State Network reproduces the correlation properties
  - for training example \( D, \tau = 100 \)
  - for unseen dynamics \( D, \tau = 30 \)

\[ \Delta_{ACF} = \sum_i |ACF_{MG} - ACF_{dESN}| \]
Autocorrelation Function

Autocorrelation function (ACF)

\[ r_\tau = \frac{c_\tau}{c_0}, \quad c_\tau = \frac{1}{N} \sum_{t=1}^{N-\tau} (x_t - \langle X \rangle)(x_{t+\tau} - \langle X \rangle) \]

- Adapted Echo State Network reproduces the correlation properties for training example D, \( \tau = 100 \)
- \( \rightarrow \) for unseen dynamics D, \( \tau = 30 \)

\[ \Delta_{ACF} = 12.43 \]

\[ \Delta_{ACF} = 10.56 \]

Does it always work?
Mackey-Glass attractors: from stable to periodic and chaotic dynamics

\[ \frac{dx}{dt} = \beta \frac{x_{\tau}}{1 + x_{\tau}^n} - \gamma x \]

- $\tau = 10$
- $\lambda_{\text{max}} > 0$

- $\tau = 20$
- $\lambda_{\text{max}} > 0$

- $\tau = 30$
Limit of long delays: phase space volume of chaotic attractor remains unaltered

\( \frac{dx}{dt} = \beta \frac{x_t}{1 + x_t^n} - \gamma x \)

\( \tau = 20 \)

\( \tau = 30 \)

\( \tau = 100 \)

\( \tau = 300 \)

\( \tau = 600 \)

\( \tau \gtrsim 10\frac{1}{\gamma} \) (condition long delay \( \tau \sim 100 \))
Training for long delays ($D, \tau = 100$) → inference works for short and long delays

Training for short delays ($D, \tau = 17$ or $30$) → inference works in the neighborhood of the training example

Knowledge of the dynamical properties useful for ML!

Autocorrelation function difference $\Delta_{ACF} = \sum_i |ACF_{MG} - ACF_{dESN}|$
Time Translational Symmetry in Delay Systems

• dynamics of the system do not change over time

• using the quasi-space representation
  • \( \rightarrow \) dynamics are independent along quasi-space \( s \)

\[
\dot{y}(t) = -y(t) + 3y(t - 100)/(1 + y(t - 100)^{10})
\]
Analogy: Delay systems - 1D Spatially Extended systems

Mackey-Glass model
\[ \dot{y}(t) = -y(t) + 3y(t - 100)/(1 + y(t - 100)^{10}) \]

Kuramoto Sivashinsky model
\[ y_t = -y y_x - y_{xx} - y_{xxxx}, \]
where \( y(x,t) \) is a scalar field
Learning one spatial extension and exploiting spatial translational symmetry enables to infer the dynamics for other spatial extensions (assuming periodic boundary conditions).

Importance of symmetries → analogy between delay and spatio-temporal systems
• **Symmetries** can be used for far reaching inferences of dynamical systems with adapted neural networks
  
  → Infer unseen/untrained dynamical regimes

• → High **generalization ability**

• **Informed machine learning** methods can tackle highly complex dynamical systems

• Plenty of **room for novel findings** at the interface between machine learning and dynamical systems

**THANK YOU**

M. Goldmann et al., “Inferring untrained complex dynamics of delay systems using an adapted echo state network”, arxiv:2111.03706