Inferring Untrained Dynamics of Complex Systems using Adapted Recurrent Neural Networks

Mirko Goldmann, Claudio R. Mirasso, Ingo Fischer, and **Miguel C. Soriano**

IFISC

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UNIT OF EXCELLENCE MARÍA DE MAEZTU

Dynamics Days Europe 2022
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- 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
Apostolos Argyris
Irene Estébanez
Moritz Pflüger
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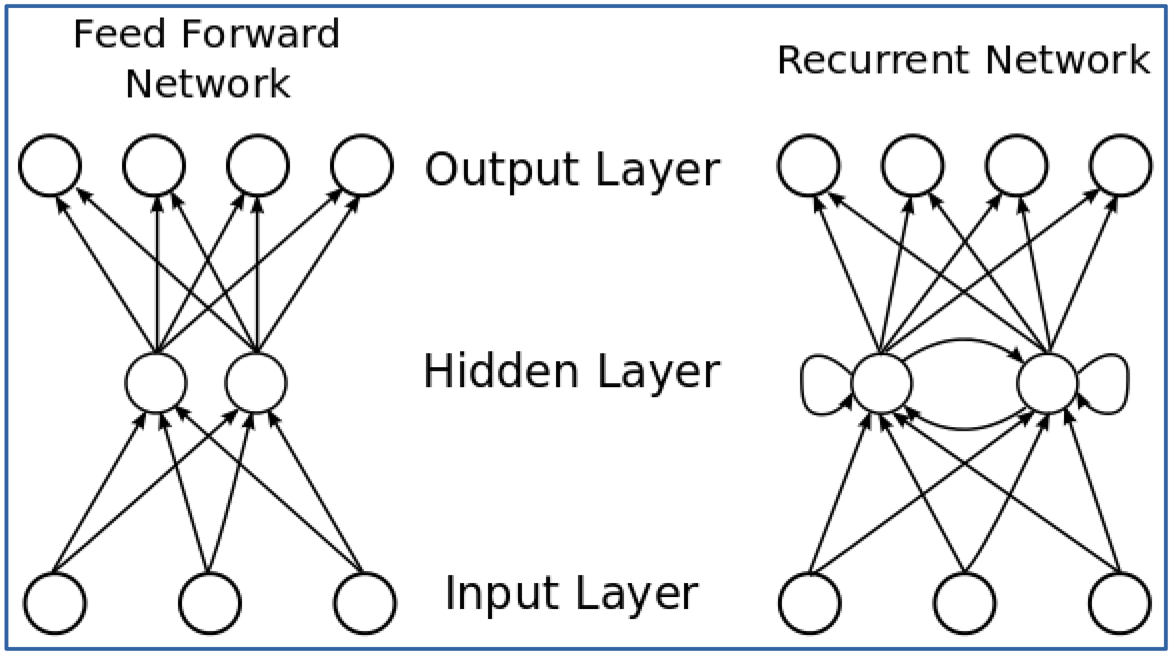
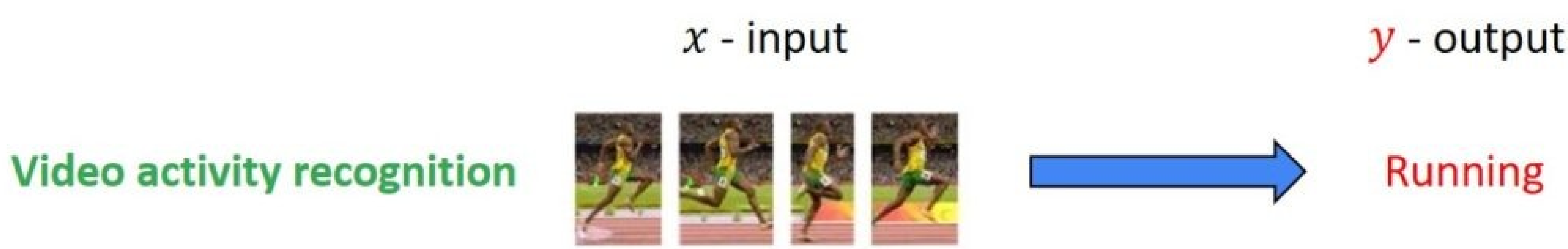
Silvia Ortín
Ingo Fischer
Jyoti P. Deka
Cap Formentor, Mallorca

Machine Learning meets Dynamical Systems

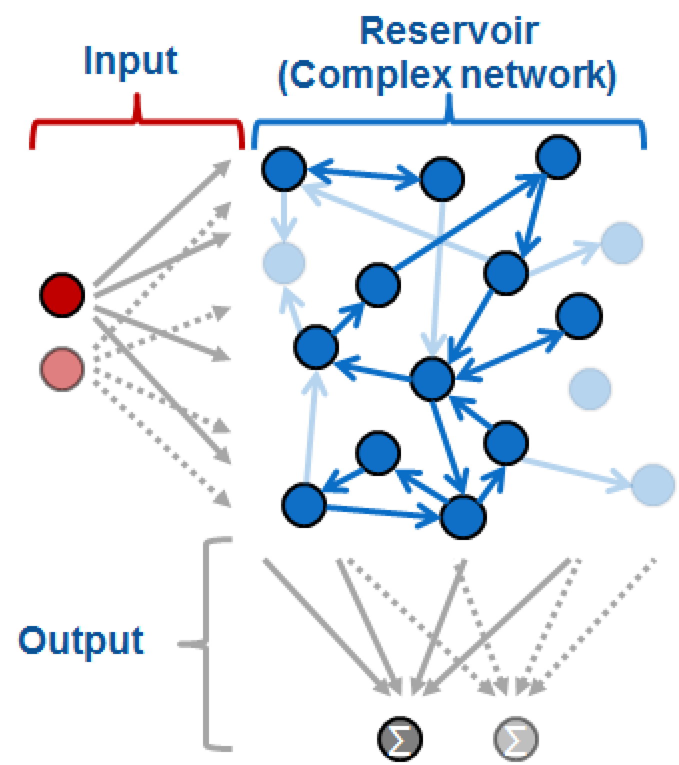


Feed forward Neural Network can approximate any continuous function (≥1 hidden layers + non-linear activations)

Recurrent Neural Networks can approximate **dynamical systems**



- 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

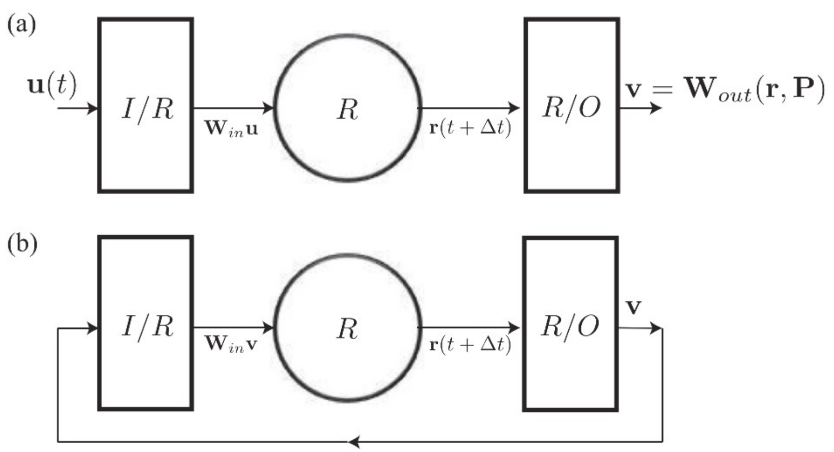


Can emulate chaotic dynamical systems!

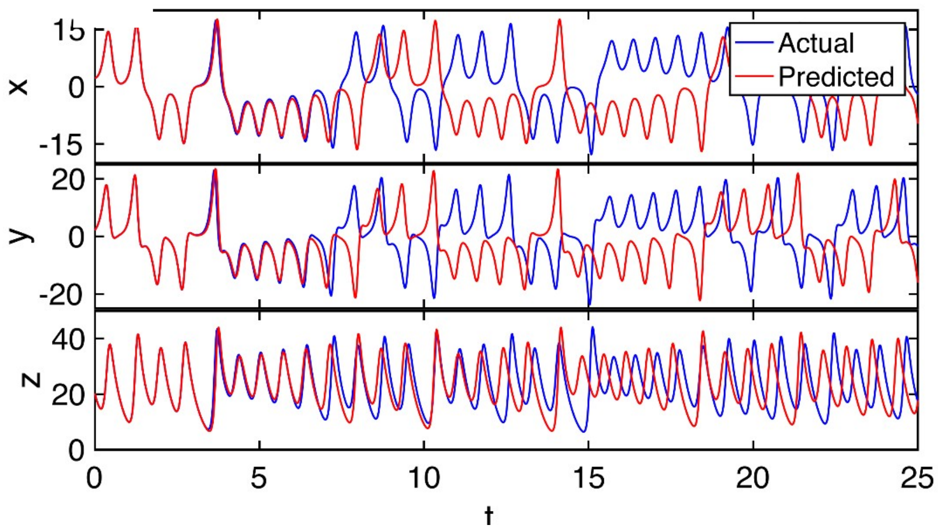
Reservoir Computing: Example

Lorenz model

$$\dot{x} = 10(y - x),$$
$$\dot{y} = x(28 - z) - y,$$
$$\dot{z} = xy - 8z/3.$$



R → Echo State Network (popular variant of RC)



	Actual Lorenz system	R1 system
Λ_1	0.91	0.90
Λ_2	0.00	0.00
Λ_3	−14.6	−10.5

J. Pathak, Z. Lu, B. R. Hunt, M. Girvan, and E. Ott. "Using machine learning to replicate chaotic attractors and calculate Lyapunov exponents from data." Chaos 27, 121102 (2017).

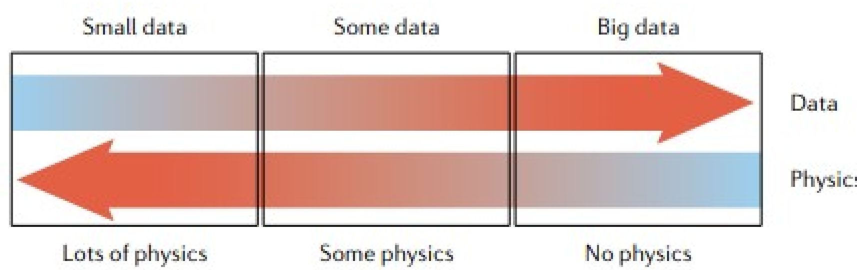
Infer unseen/untrained dynamics of systems by learning from a single example?

- 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



G. E. Karniadakis et al., “Physics-informed machine learning.” Nature Reviews Physics 3, 422-440 (2021).

Delay Systems

$$\dot{x}(t) = F\left(x(t), x(t-\tau); p\right)$$

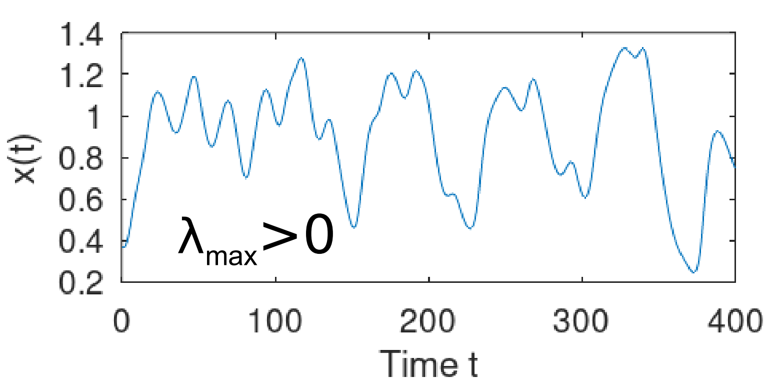
- delays appear where signal propagation is finite
  - neuroscience, photonics, epidemiologic models and control problems

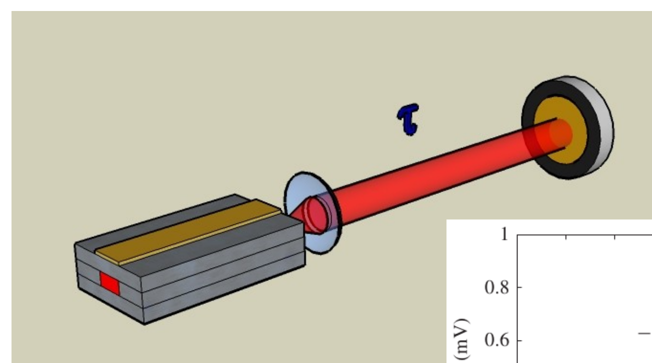
- rely on a continuous history function
  - infinite dimensional

$$h \in [-\tau, 0]$$

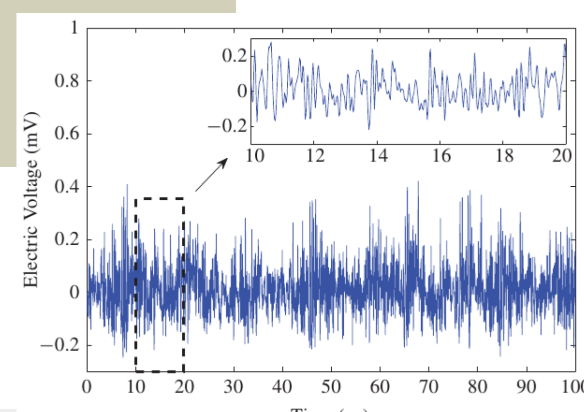
- for long delays these systems can become chaotic

Mackey-Glass system





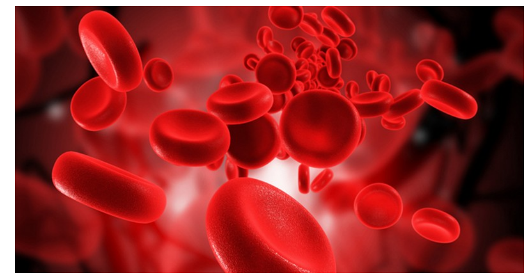
SL with feedback



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)

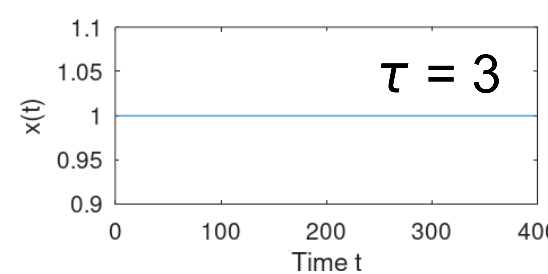
- x: concentration (assumed non-negative for all times) of circulating blood cells
- β, γ and n: constants controlling the production of these cells
- x_τ , $x(t\text{-}\tau)$

For some intermediate values of x_τ the production rate would be adequate

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

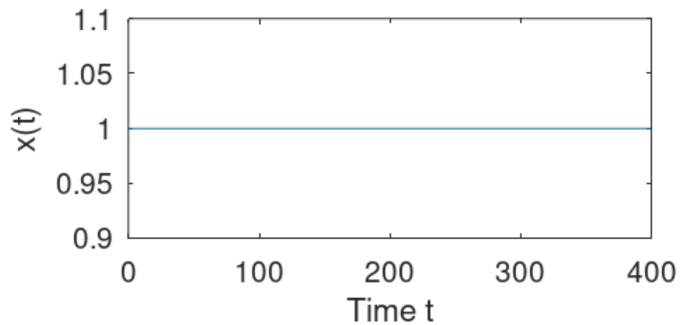
If $1\ll x_\tau$ person would have too many blood cells so that the production rate would once again be low

$\beta=0.2$, $\gamma=0.1$ and $n=10$

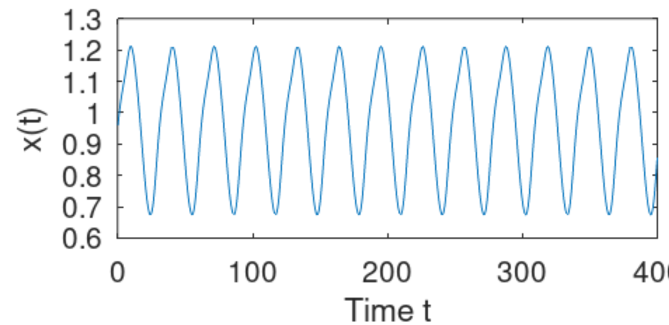


Leon Glass and Michael Mackey (2010), Scholarpedia, 5(3):6908.

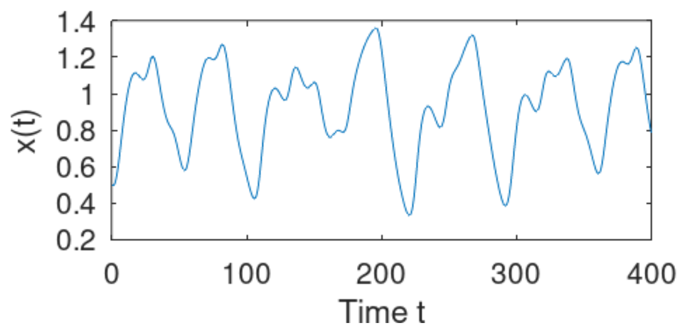
$\tau = 3$



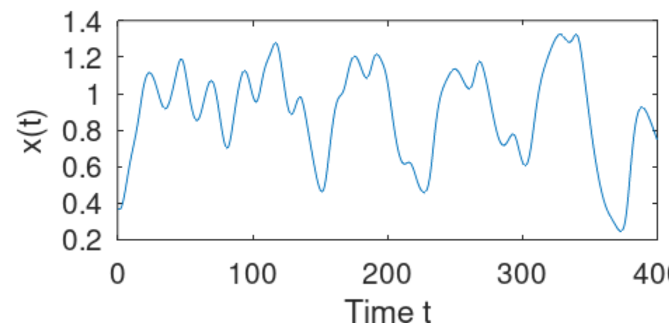
$\tau = 10$



$\tau = 20$

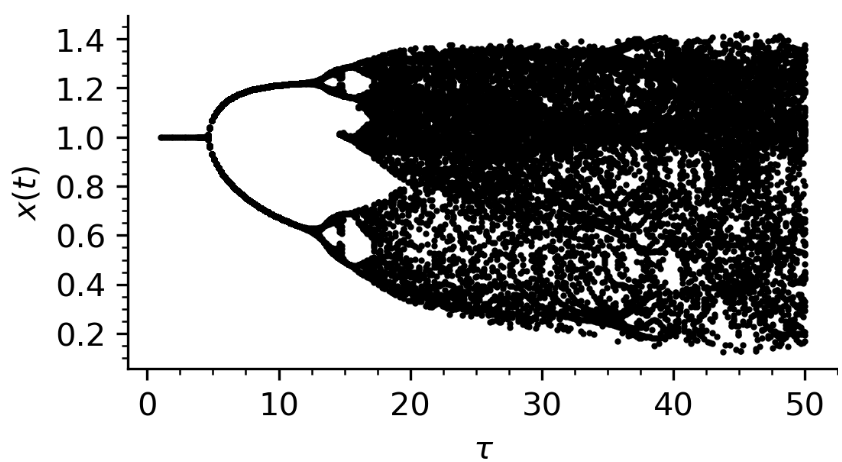


$\tau = 30$



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

β=0.2, γ=0.1 and n=10



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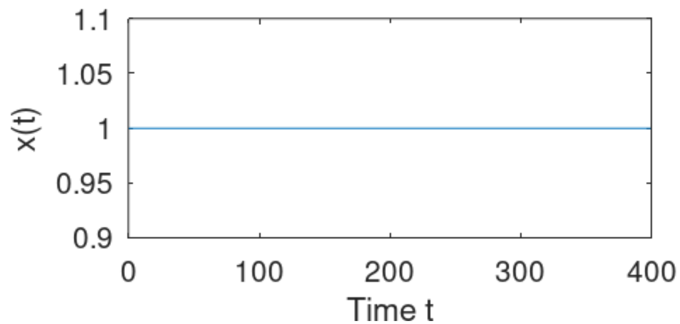

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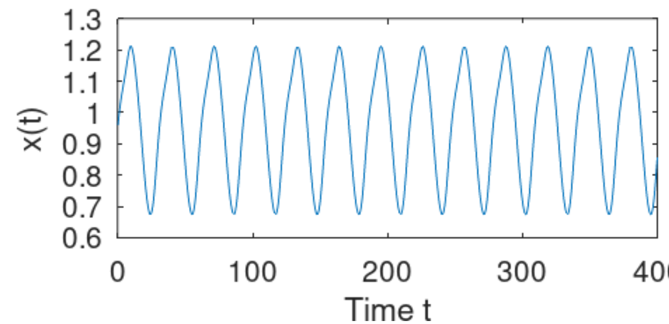

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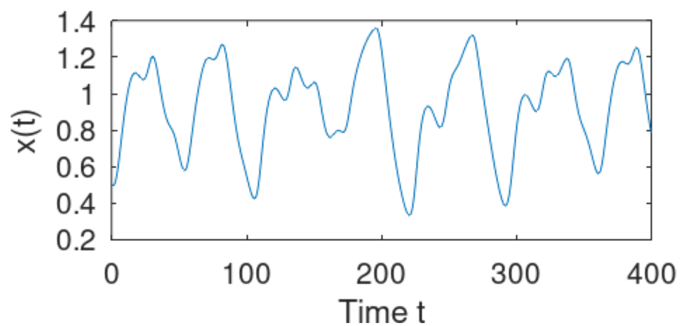
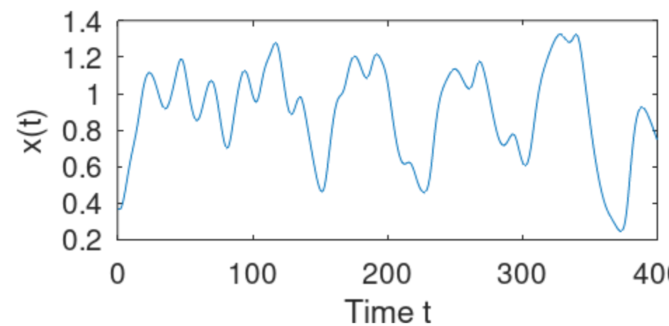
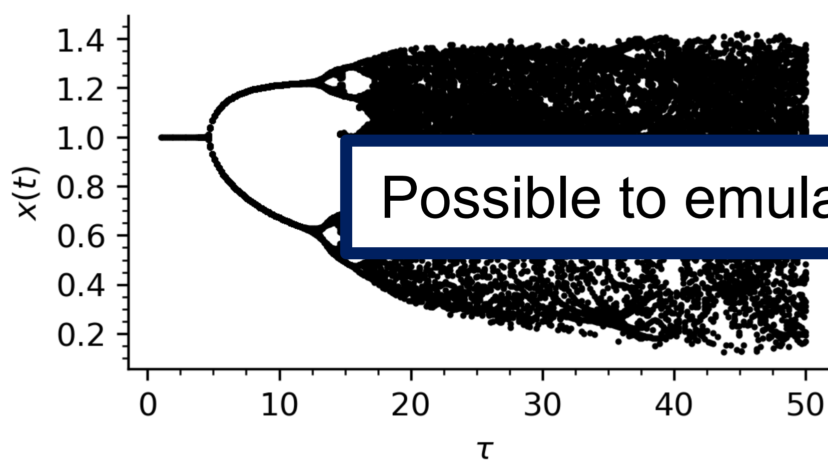


$\tau = 30$



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

β=0.2, γ=0.1 and n=10

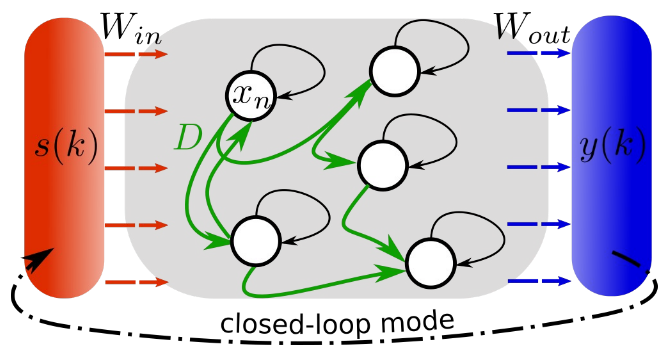


Possible to emulate with ML?

Delayed Echo State Networks

Incorporate a delay into the neural network

$$\vec{x}(n+1) = \alpha\vec{x}(n) + \beta\tanh(\mathbf{W}\vec{x}(n-D) + \gamma\mathbf{W}_{in}s(n) + \mathbf{W}_b)$$

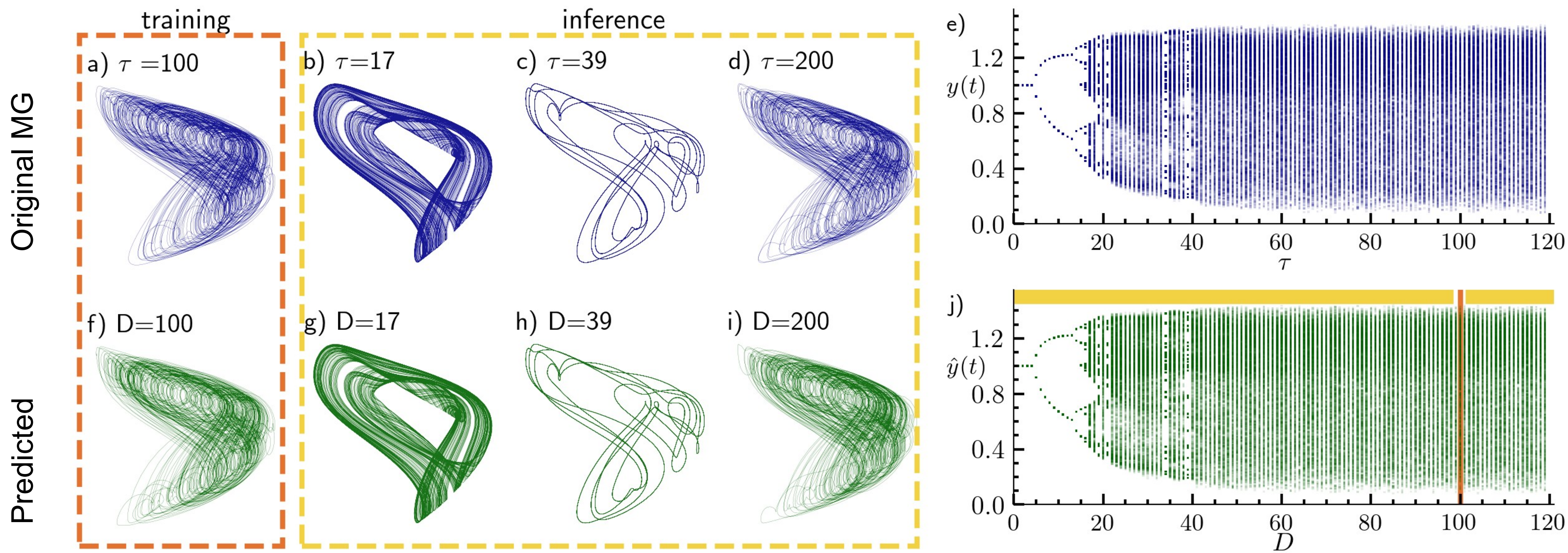


Optimal prediction performance for data of Mackey Glass system (τ) at D=τ

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

$$\vec{x}(n+1) = \alpha\vec{x}(n) + \beta\tanh(\mathbf{W}\vec{x}(n-D) + \boxed{\gamma\mathbf{W}_{in}W_{out}x(n)} + \mathbf{W}_b)$$

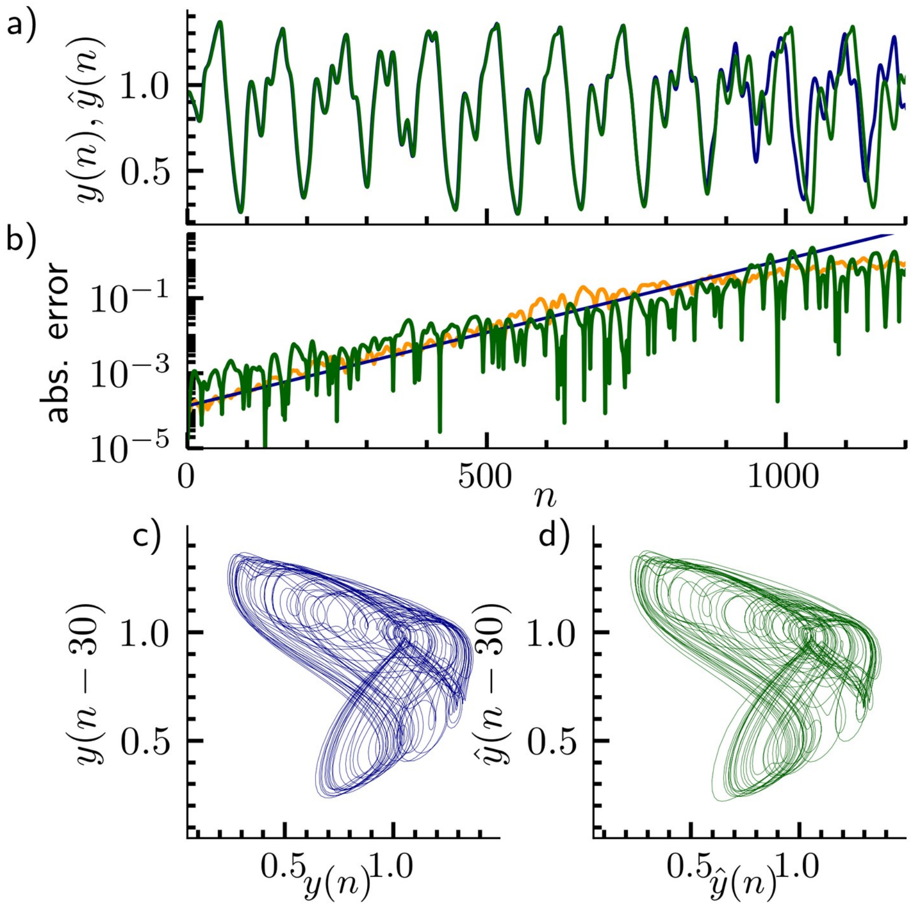
After training reconfigure network by setting delay D to untrained values
→ Inferring unseen dynamical regimes

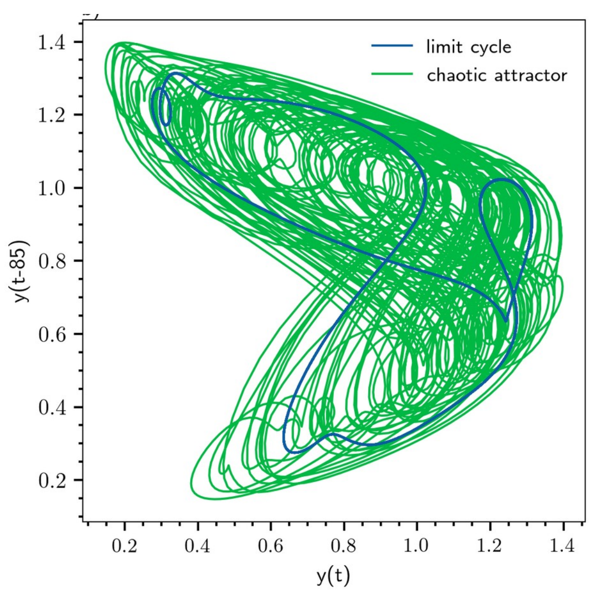


- Training for a long delay D, τ = 100
- After training scanning D
- Learning one size enables to infer the entire bifurcation diagram

Possible to emulate with ML!

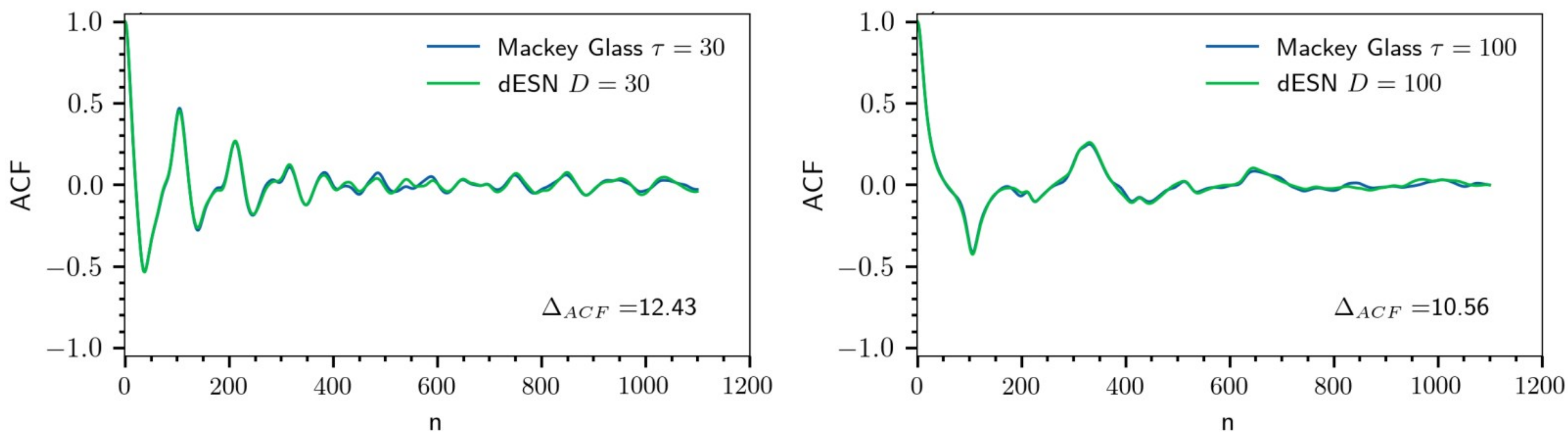
- Training at a delay of D=100
  - † After training: reducing the delay length to D=30
  - † Inference reveals unseen/untrained chaotic attractor
  - † Lyapunov exponent can be precisely derived from the reservoir
- Method even reveals multistabilities of the Mackey-Glass system





Autocorrelation function (ACF)

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

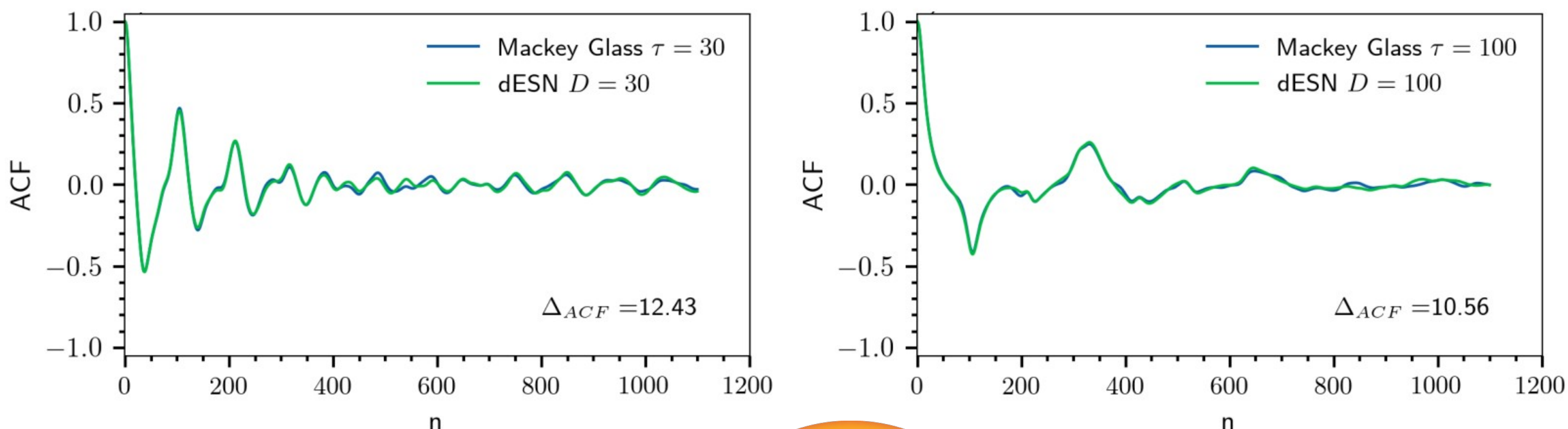


- Adapted Echo State Network reproduces the correlation properties
  - → for training example D, τ = 100
  - → for unseen dynamics D, τ = 30

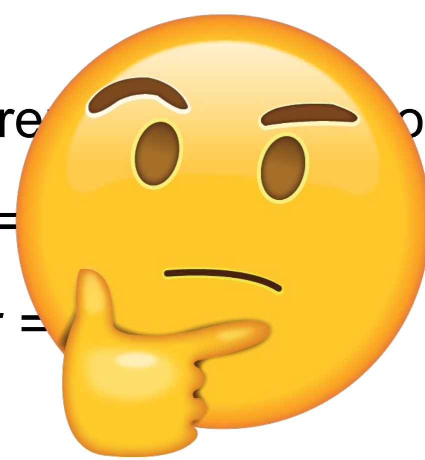
$$\Delta_{ACF} = \sum_i |ACF_{MG} - ACF_{dESN}|$$

Autocorrelation function (ACF)

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



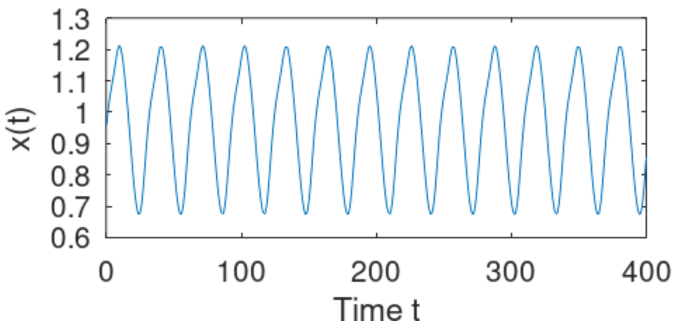
- Adapted Echo State Network re orrelation properties
  - → for training example D, τ =
  - → for unseen dynamics D, τ =

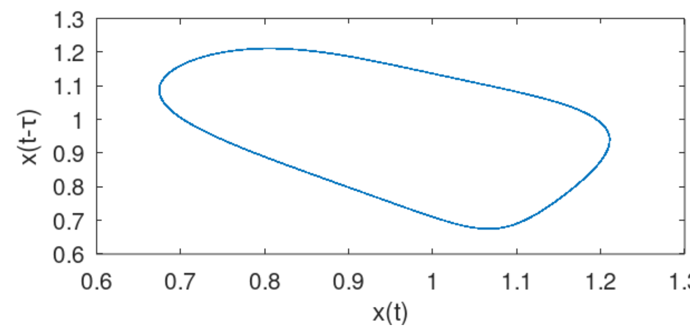


Does it always work?

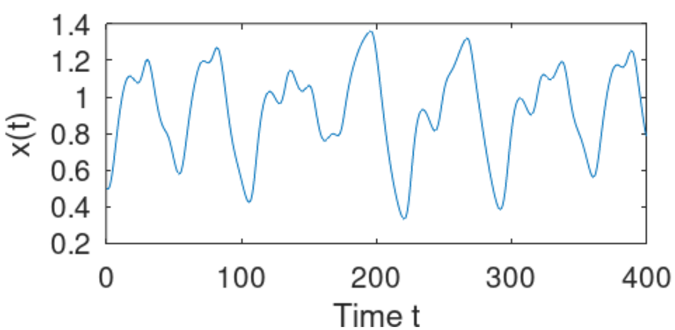
Mackey-Glass attractors: from stable to periodic and chaotic dynamics

$\tau = 10$

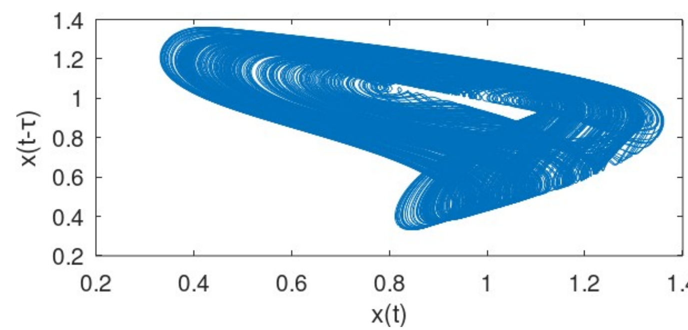




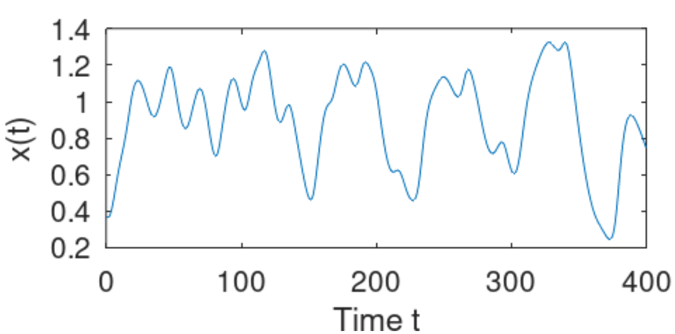
$\tau = 20$



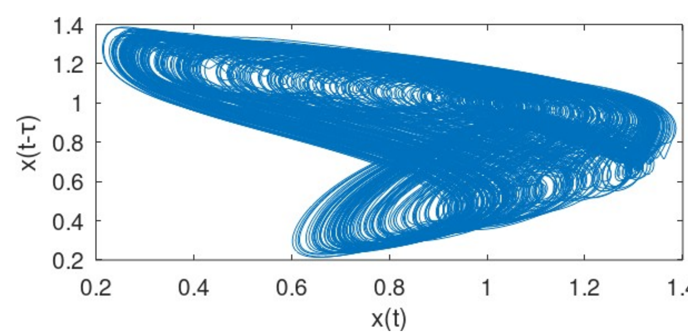
$\lambda_{max} > 0$



$\tau = 30$

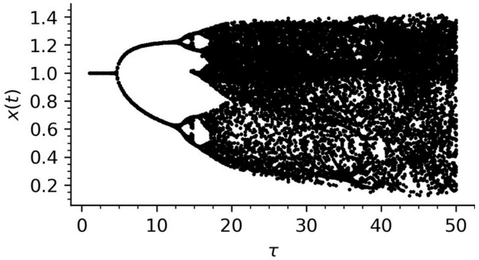


$\lambda_{max} > 0$



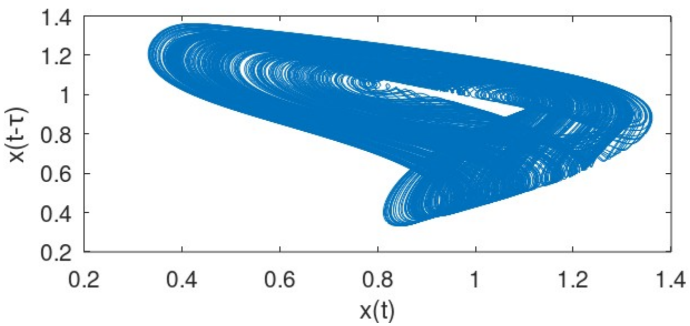
$$\frac{dx}{dt} = \beta \frac{x_\tau}{1 + x_\tau{}^n} - \gamma x$$

Long delay vs. short delay

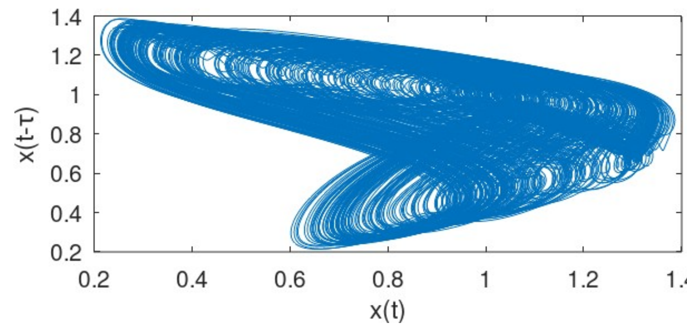


Limit of long delays: phase space volume of chaotic attractor remains unaltered

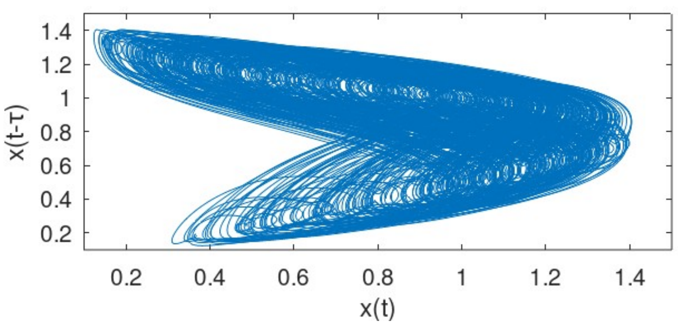
$\tau = 20$



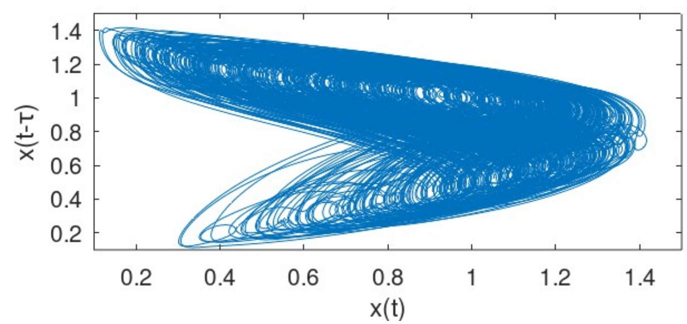
$\tau = 30$



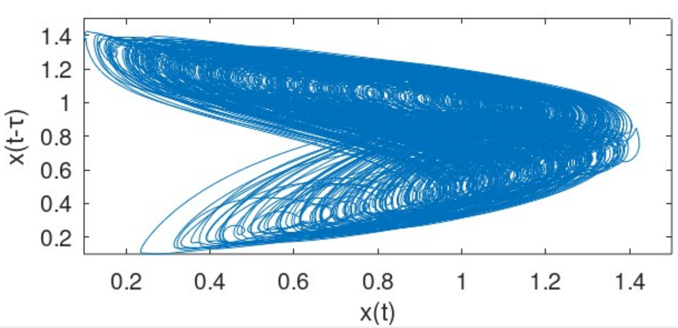
$\tau = 100$



$\tau = 300$

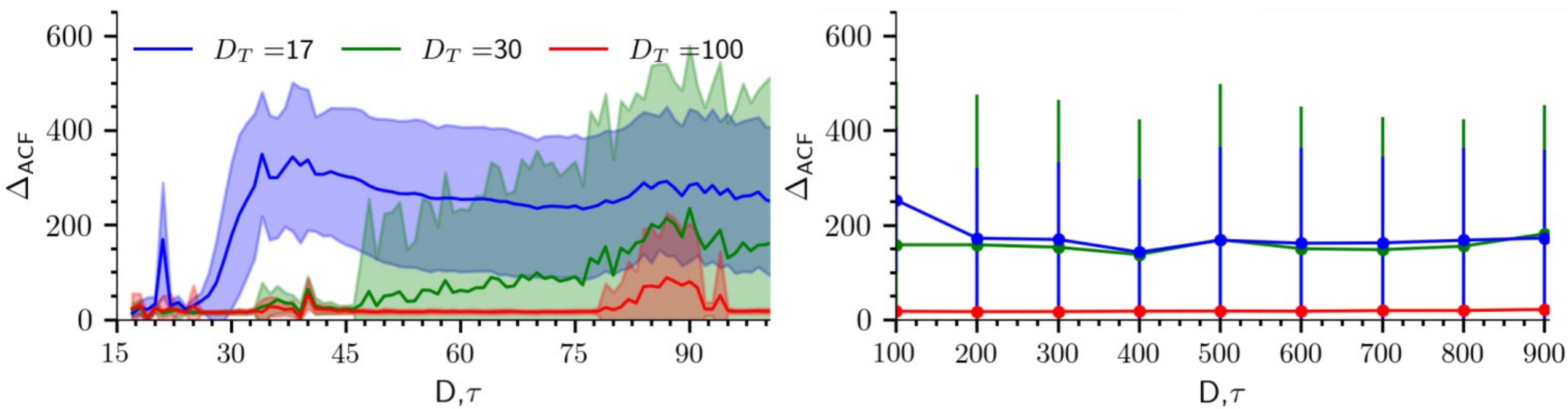


$\tau = 600$



$$\tau \gtrsim 10 \frac{1}{\gamma}$$ (condition long delay $\tau \sim 100$)

Autocorrelation function difference $\Delta_{ACF} = \sum_i |ACF_{MG} - ACF_{dESN}|$

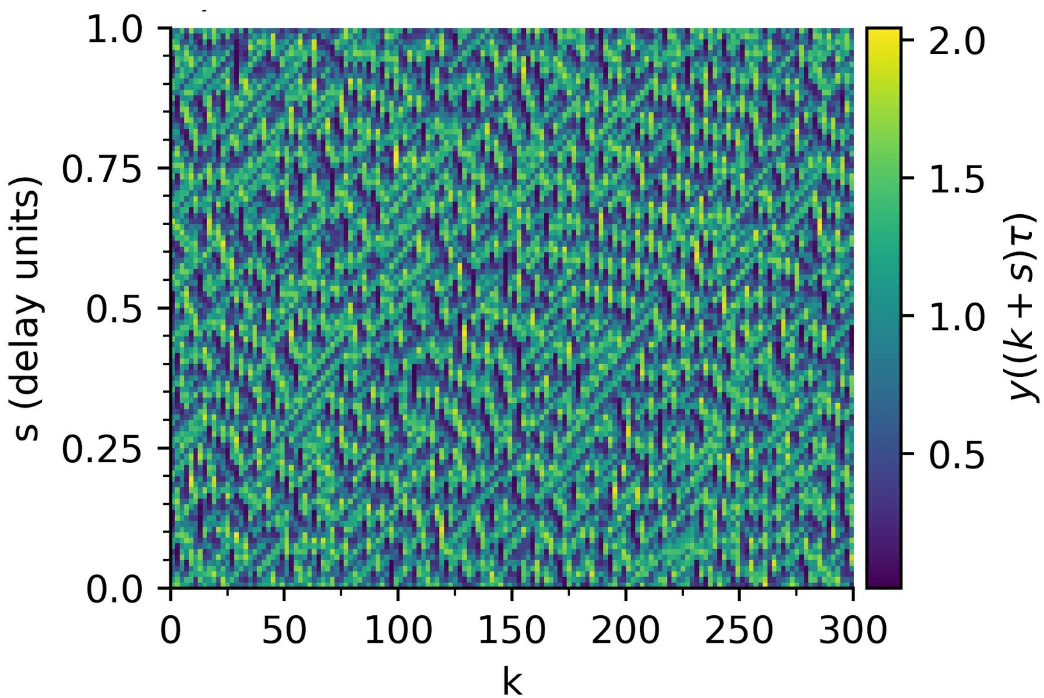


- Training for long delays (D,τ = 100) → inference works for short and long delays
- Training for short delays (D,τ = 17 or 30) → inference works in the neighborhood of the training example

Knowledge of the dynamical properties useful for ML!

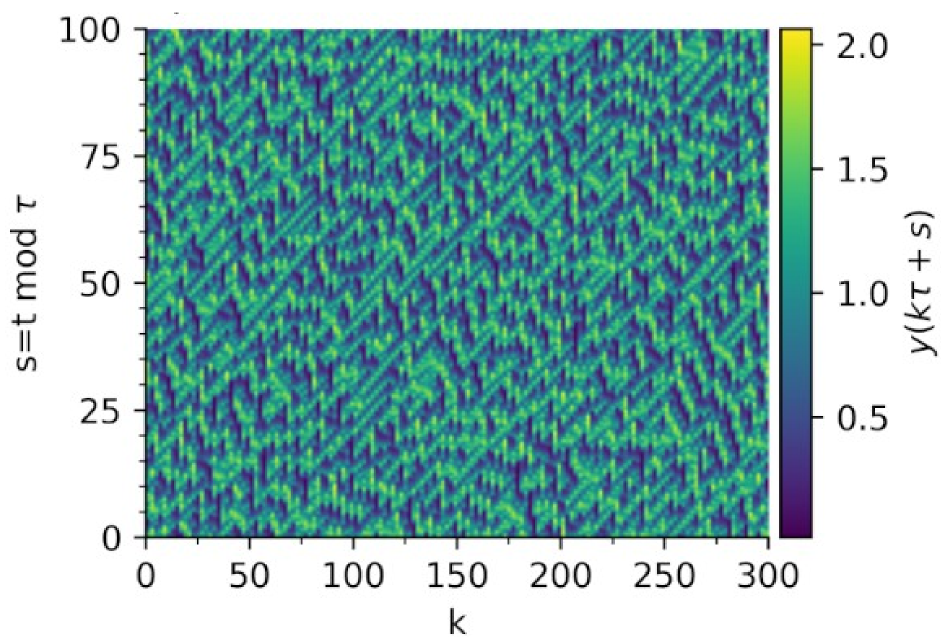
Time Translational Symmetry in Delay Systems

- dynamics of the system do not change over time
- using the quasi-space representation
  - → dynamics are independent along quasi-space s



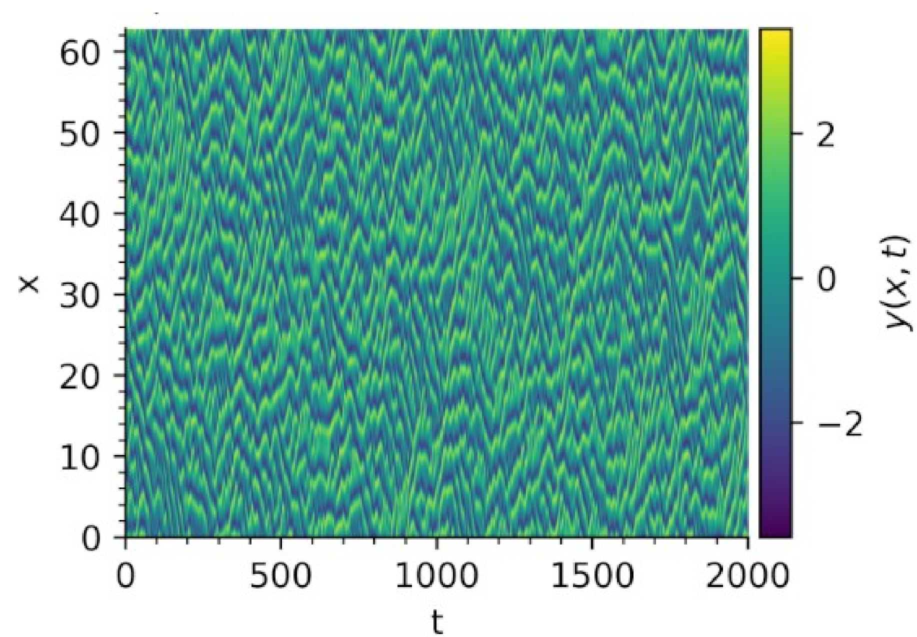
$$\dot{y}(t) = -y(t) + 3y(t-100)/(1+y(t-100)^{10})$$

Analogy: Delay systems - 1D Spatially Extended systems



Mackey-Glass model

$$\dot{y}(t) = -y(t) + 3y(t-100)/(1+y(t-100)^{10})$$

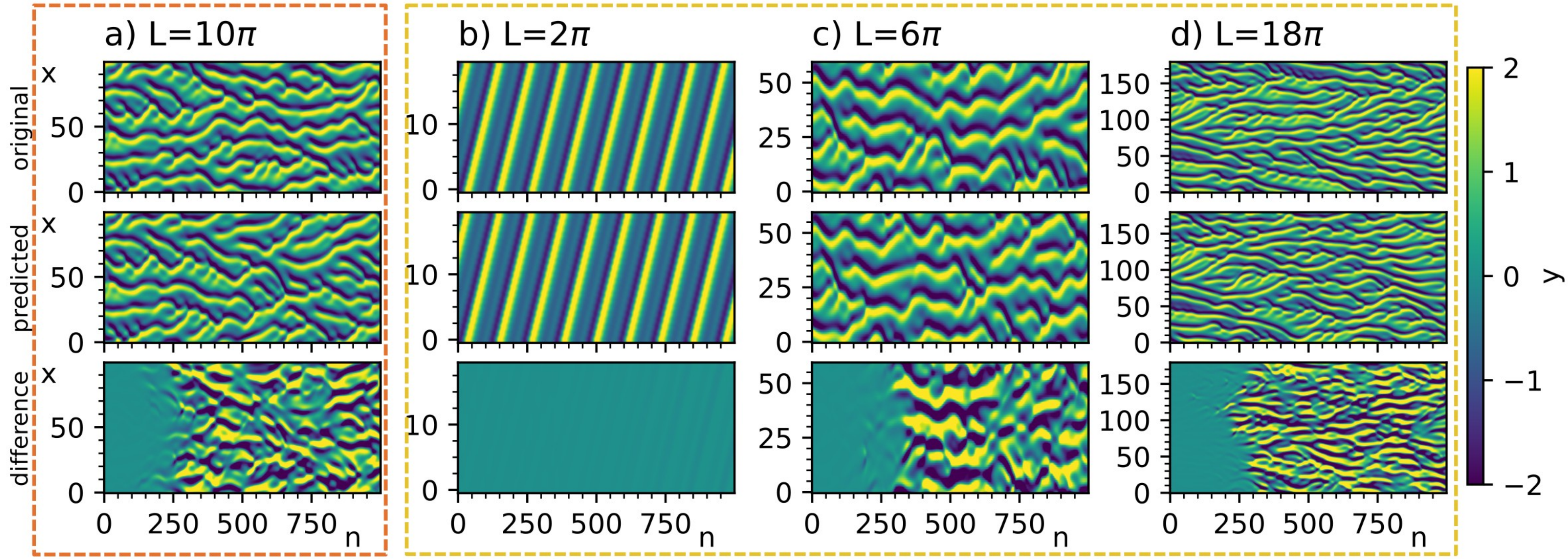


Kuramoto Sivashinsky model

$$y_t = -yy_x - y_{xx} - y_{xxxx},$$

where $y(x,t)$ is a scalar field

Inferring untrained dynamics of a Kuramoto Sivashinsky model



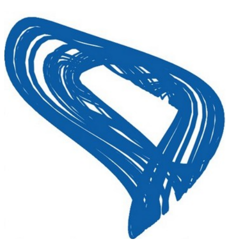
- Learning one spatial extension and exploiting spatial translational symmetry enables to infer the dynamics for other spatial extensions (assuming periodic boundary conditions)
- Importance of symmetries → analogy between delay and spatio-temporal systems

- **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
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