a Neural Network Approach to Learn Delay Differential Equations via Pseudospectral Collocation

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introducing DDEs [3, 5, 6]

- let $\tau > 0$, $X \coloneqq C([-\tau, 0]; \mathbb{R})$ and consider

$$x'(t) = f(x_t)$$

  for smooth $f : X \to \mathbb{R}$ and $x_t(\theta) \coloneqq x(t + \theta)$, $\theta \in [-\tau, 0]$

- e.g., Mackey-Glass [9]:

$$f(\varphi) \coloneqq \frac{\beta\varphi(-\tau)}{1 + \varphi(-\tau)^n} - \gamma\varphi(0) \quad \Rightarrow \quad x'(t) = \frac{\beta x(t - \tau)}{1 + x(t - \tau)^n} - \gamma x(t)$$

(in all the experiments: $\beta = 4, \gamma = 2, n = 9.6, \tau = 1$)

[5] Hale – Springer 1977
[3] Diekmann, van Gils, Verduyn Lunel, Walther – Springer 1995
[6] Erneux – Springer 2009
[9] Mackey, Glass – Science 1977
(full references at the end)

the abstract Cauchy problem [4]

- the IVP in $\mathbb{R}$

$$\begin{cases} x'(t) = f(x_t), & t \geqslant 0 \\ x(\theta) = \varphi(\theta), & \theta \in [-\tau, 0], \end{cases}$$

is equivalent to the IVP in X

$$\begin{cases} u'(t) = \mathcal{A}(u(t)), & t \geqslant 0, \\ u(0) = \varphi \end{cases} \tag{1}$$

through $u(t) = x_t$ for $\varphi \in \mathcal{D}(\mathcal{A})$, where $\mathcal{A} : \mathcal{D}(\mathcal{A}) \subseteq X \to X$ given by

$$\mathcal{A}(\psi) = \psi', \quad \mathcal{D}(\mathcal{A}) = \{\psi \in X \ : \ \psi' \in X \text{ and } \psi'(0) = f(\psi)\}$$

generates the associated semigroup $\{T(t)\}_{t \geqslant 0}$ of solution operators

$$T(t) : X \to X, \qquad T(t)\varphi \coloneqq x_t$$

- DDEs give rise to dynamical systems on X, hence ∞-dimensional:
  - a general approach: reduce (1) to a system of ODEs + tools for ODEs
  - [7] uses Euler in view of applying NODEs and TDNNs to learn DDEs

[4] Engel, Nagel – Springer 1999
[7] Ji, Orosz – IFAC PoL 2022

PseudoSpectral Collocation (PSC)

- let $-\tau = \theta_M < \cdots < \theta_1 < \theta_0 = 0$ be Chebyshev extrema
- for $X_M \coloneqq \mathbb{R}^{M+1}$ set
  - $R_M : X \to X_M$, $\quad R_M\psi \coloneqq (\psi(\theta_0), \psi(\theta_1), \ldots, \psi(\theta_M))$
  - $P_M : X_M \to X$, $\quad (P_M\Psi)(\theta) \coloneqq \sum_{j=0}^{M} \ell_j(\theta)\Psi_j,\ \theta \in [-\tau, 0]$
- discretize $\mathcal{A} : \mathcal{D}(\mathcal{A}) \subseteq X \to X$

$$\mathcal{A}\psi = \psi', \quad \mathcal{D}(\mathcal{A}) = \{\psi \in X \ :\ \psi' \in X \ \text{ and } \ \psi'(0) = f(\psi)\}$$

with $\mathcal{A}_M : X_M \to X_M$

$$[\mathcal{A}_M(\Psi)]_{i=1,\ldots,M} = [R_M(P_M\Psi)']_{i=1,\ldots,M}, \quad [\mathcal{A}_M(\Psi)]_0 = f(P_M\Psi)$$

[2] B., Maset, Vermiglio – SISC 2005 $\rightarrow$ f linear

[1] B., Diekmann, Gyllenberg, Scarabel, Vermiglio – SIADS 2016 $\rightarrow$ f nonlinear

from DDEs to ODEs

- let
$$U(t) \coloneqq (U_0(t), U_1(t), \ldots, U_M(t))^T \in X_M, \qquad U_i(t) \approx u(t)(\theta_i)$$
- the abstract Cauchy problem
$$\begin{cases} u'(t) = \mathcal{A}(u(t)), & t \geqslant 0, \\ u(0) = \varphi \end{cases}$$
with
$$\mathcal{A}\psi = \psi', \quad \mathcal{D}(\mathcal{A}) = \{\psi \in X \ : \ \psi' \in X \ \text{ and } \ \psi'(0) = f(\psi)\}$$
is reduced to the $M+1$ ODEs
$$\begin{cases} U_0'(t) = f(P_M U(t)) \\ U_i'(t) = [D_M U(t)]_i, & i = 1, \ldots, M, \\ U(0) = (\varphi(\theta_0), \varphi(\theta_1), \ldots, \varphi(\theta_M))^T \end{cases}$$
for $[D_M]_{i,j} \coloneqq \ell_j'(\theta_i)$, $i = 1, \ldots, M$, $j = 0, 1, \ldots, M$
- the RHS f affects only the first ODE: easy to code [8]

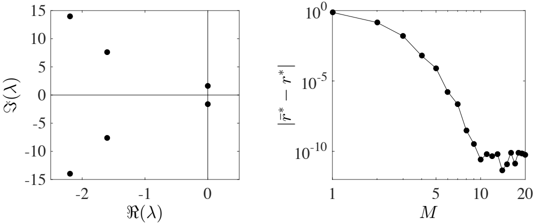
[8] Liessi, Santi, Vermiglio – IFAC TDS 2022

a simple test

- the logistic DDE

$$x'(t) = rx(t)[1 - x(t-1)]$$

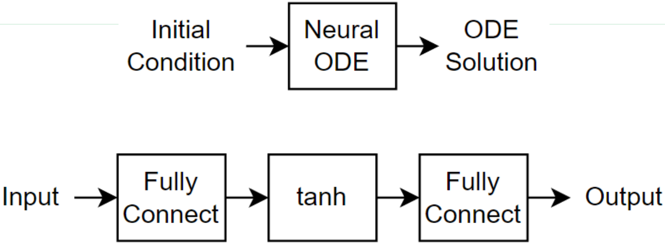
  has equilibrium $\bar{x} = 1$ for all r:
  - asymptotically stable for $r \in (0, \pi/2)$
  - unstable for $r > \pi/2$
  - Hopf bifurcation at $r^* := \pi/2$
- error in approximating r^* via `MatCont` on approximating ODE:



Neural ODEs [10]

NODEs are deep learning operations whose output is defined by the (numerical) solution of an associated ODE:

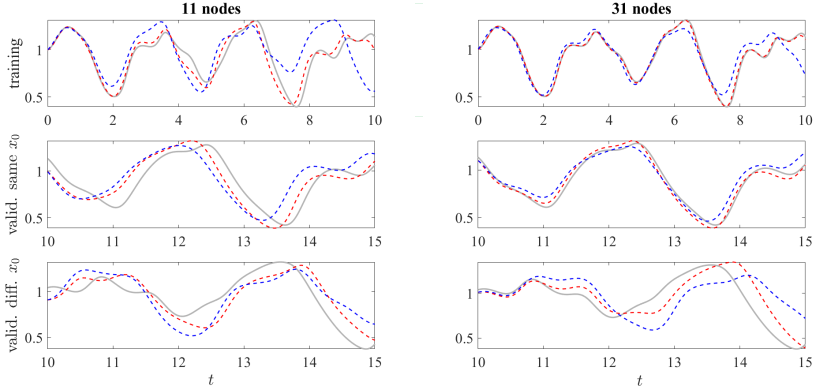
$$y' = g(t, y, \theta)$$



Implementation: We use MATLAB tools for DL (e.g., `dlarray`, `dlode45`)

[10] Chen, Bettencourt, Rubanova, Duvenaud – NeurIPS 2018

ODEs from DDEs via Euler

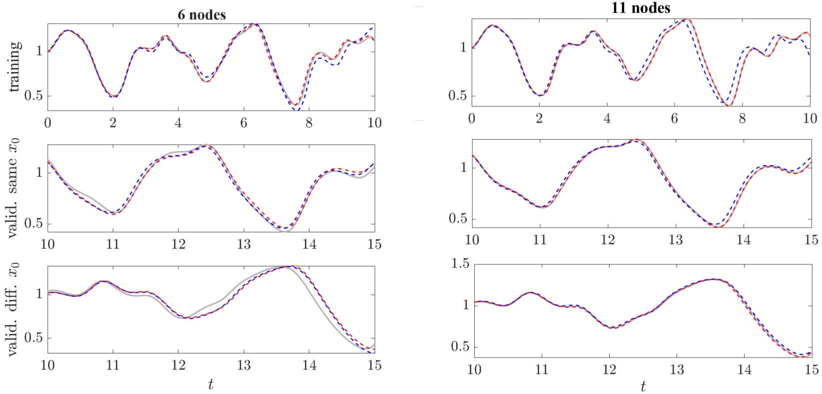


grey: ground truth DDE, red: ground truth ODE, blue: NODE

CPU times:

Euler: 9 minutes for 11 nodes, 12 m for 31 nodes

ODEs from DDEs via PSC



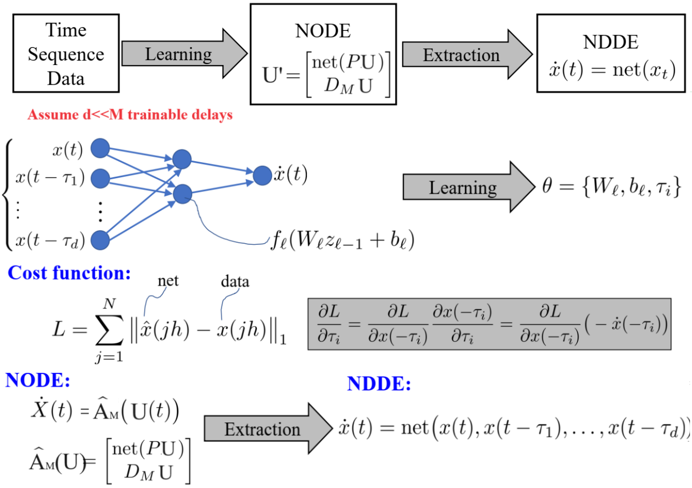
grey: ground truth DDE, red: ground truth ODE, blue: NODE

CPU times:

PSC: 9 minutes for 6 nodes, 9m for 11 nodes

Time delay neural networks [11]

TDNNs are capable of handling delayed input sequences



[11] Waibel, Hanazawa, Hinton, Shikano, Lang – IEEE TASSP (1989)

Resume

ODE:

$$U'(t) = \begin{bmatrix} \frac{\beta U_M(t)}{1+(U_M(t))^n} - \gamma U_0(t) \\ D_M U(t) \end{bmatrix}$$

NODE:

$$U'(t) = \begin{bmatrix} W_3 \tanh(W_2 \tanh(W_1 P U(t) + b_1) + b_2) \\ D_M U(t) \end{bmatrix}$$

NDDE:

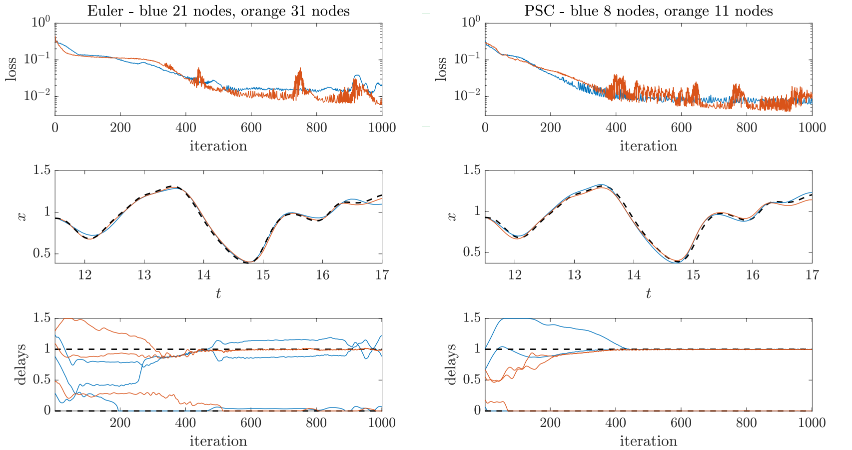
$$x'(t) = W_3 \tanh(W_2 \tanh(W_1 \begin{bmatrix} x(t) \\ x(t-\tau_1) \\ \dots \\ x(t-\tau_d) \end{bmatrix} + b_1) + b_2),$$

Here $P : \mathbb{R}^{M+1} \to \mathbb{R}^{d+1}$ transforms state collocated samples $(x(t+\theta_0), \dots, x(t+\theta_M))$ into delayed states $(x(t), x(t-\tau_1), \dots, x(t-\tau_d))$ and is computed through barycentric interpolation [12] on Chebyshev extrema

Info: simulation horizon = 0.5, batch size = 1000, and update parameters using adaptive moment estimation method

[12] J. Berrut, L. Trefethen – SIAM review 2004

TDNN Results



CPU times:

- Euler: 16 minutes for 21 nodes, 17m for 31 nodes
- PSC: 8m for 8 nodes, 10m for 11 nodes

SINDy [13] for DDEs

- Collect measurement data $\mathbf{x}(t)$ and (approximate) $\mathbf{x}'(t)$
- Construct a library $\Theta(\mathbf{x})$ of candidate functions
- Solve $\mathbf{x}' = \Theta(\mathbf{x})\boldsymbol{\Xi}$ by sparse regression promoting the sparsity of $\boldsymbol{\Xi}$

"Expert" SINDy for DDEs [14, 15]

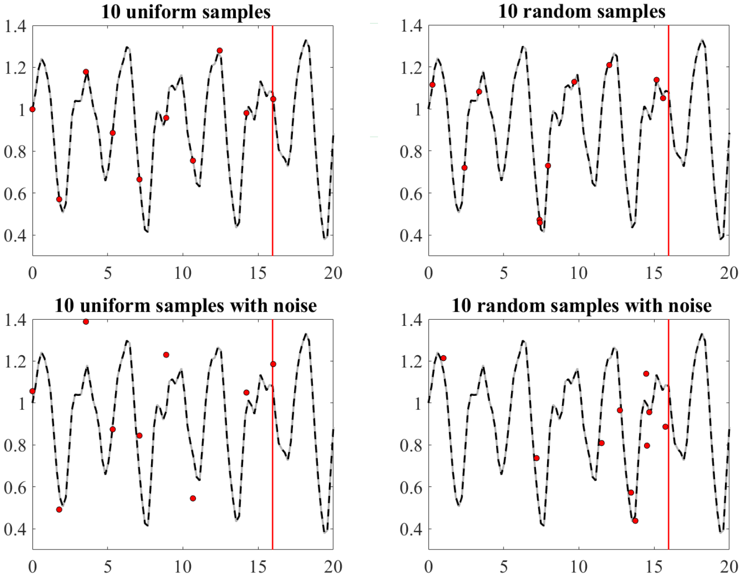
- direct on the DDE
- via library extension to the delayed data-set $x(t - \tau_i)$
- delays assumed to be known

"Pragmatic" SINDy for DDEs

- on ODEs via PSC of the DDE
- via library extension to the collocated data-set $x(t + \theta_i)$
- delays assumed not to be known

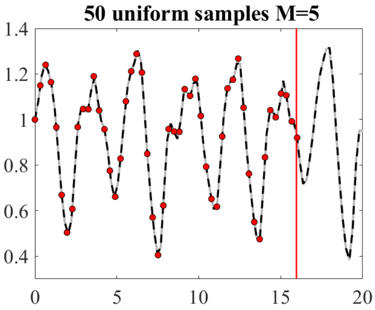
[13] Brunton, Proctor, Kutz – PNAS (2016)
[14] Breda, Demo, Pecile, Rozza – IFAC TDS 2022
[15] Sandoz, Ducret, Gottwald, Vilmart, Perron – PMPES 2023

Expert SINDy



grey: ground truth, black: SINDy, red: samples

Pragmatic SINDy



Concluding remarks

- data-driven methods for DDEs
- Need to explore and understand more
- Challenge: handling of delay terms
- ongoing and future:
  - SINDy for stochastic DDEs, with R. D'Ambrosio (L'Aquila), D. Conte and I. Santaniello (Salerno)
  - extend to structured population models (PNRR)

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