Neural Delay Differential Equations

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Why Neural Delay Differential Equations (NDDEs)

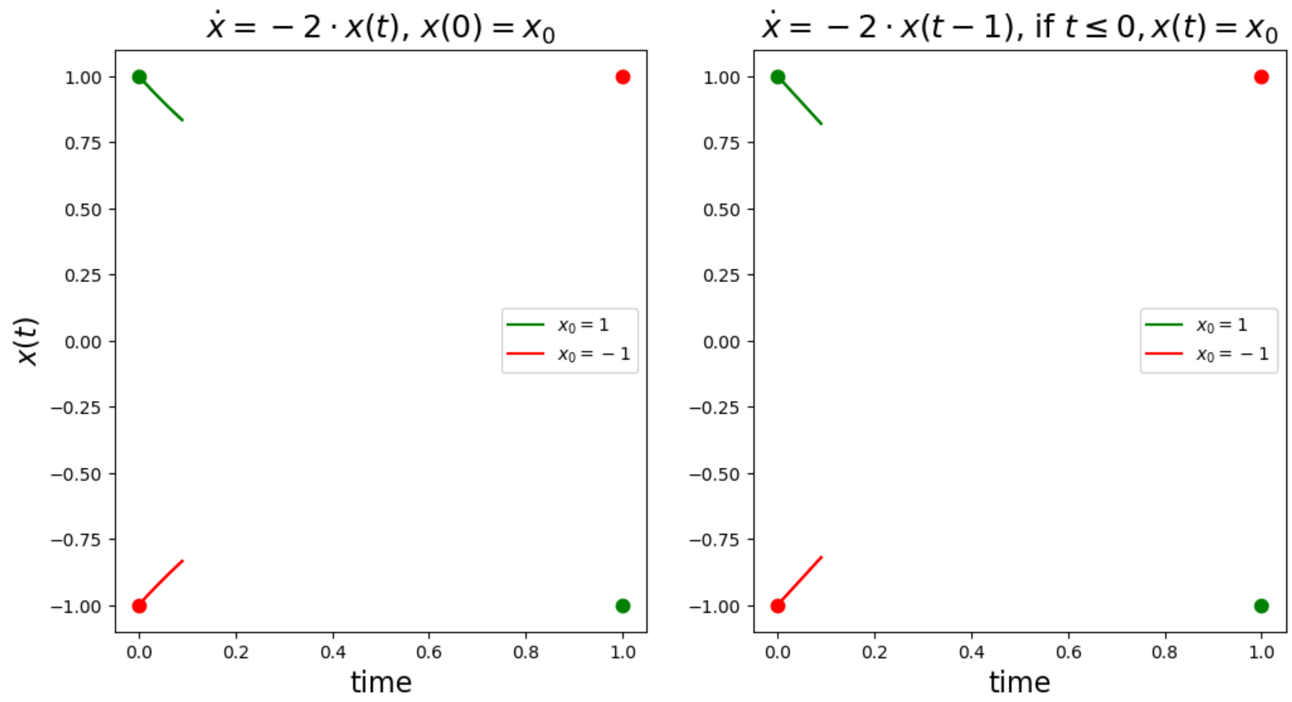
- Neural Ordinary Differential Equations (NODEs) are not universal, cannot represent some maps, such as the ***reflections*** or the ***concentric annuli***
- NODEs are not suitable to model the underlying system with the delay effect, such as **Mackey-Glass system**

Dupont et al., Augmented neural odes. **NeurIPS** 2019
Zhang et al., Approximation capabilities of neural odes and invertible residual networks. **ICML** 2020
Mackey, M. and Glass, L. Oscillation and chaos in physiological control systems. **Science**, 1977

Limitations of Neural ODEs

Dupont et al., Augmented Neural ODEs, NeurIPS, 2019: $g_{1d}(1) = -1,$ $g_{1d}(-1) = 1$ ***reflections***

Proposition 1. *The flow of an ODE cannot represent* $g_{1d}(x)$.



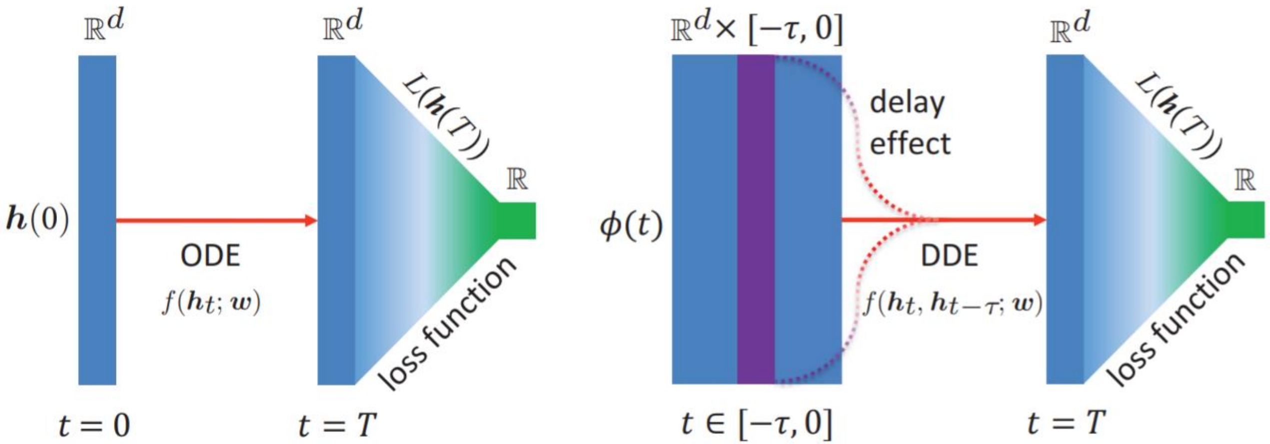
Neural Delay Differential Equations (NDDEs)

- Neural Ordinary Differential Equations (ODEs):

$$\frac{\mathrm{d}h(t)}{\mathrm{d}t} = f(h(t), w),\ h(0) = h_0$$

- Neural Delay Differential Equations (DDEs):

$$\frac{\mathrm{d}h(t)}{\mathrm{d}t} = f(h(t), h(t-\tau), w),\ if\ t \leq 0, h(t) = h_0$$



Universal approximation and adjoint dynamics of NDDEs

Theorem 2 *(Universal approximating capability of the NDDEs). For any given continuous function* $F : \mathbb{R}^n \to \mathbb{R}^n$*, if one can construct a neural network for approximating the map* $G(\boldsymbol{x}) = \frac{1}{T}[F(\boldsymbol{x}) - \boldsymbol{x}]$*, then there exists an NDDE of* n*-dimension that can model the map* $\boldsymbol{x} \mapsto F(\boldsymbol{x})$*, that is,* $h(T) = F(\boldsymbol{x})$ *with the initial function* $\phi(t) = \boldsymbol{x}$ *for* $t \leq 0$.

Adjoint: $\lambda(t) = \frac{\partial L(x(T))}{\partial x(t)}$

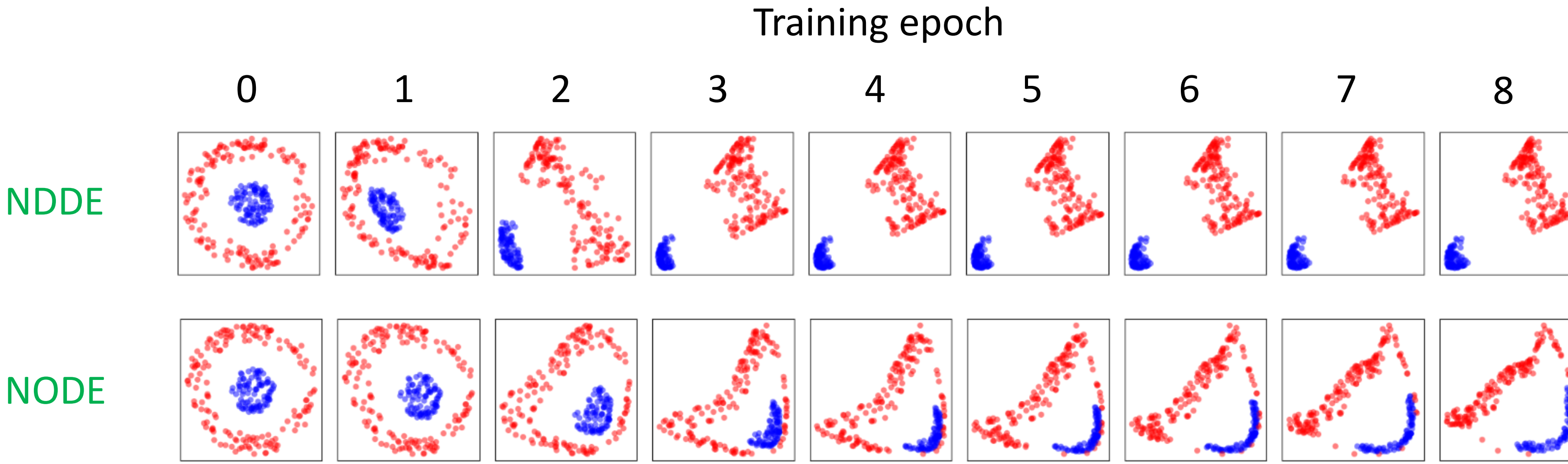
Theorem 1 *(Adjoint method for NDDEs). Consider the loss function* $L(\cdot)$*. Then, the dynamics of adjoint can be written as*

$$\begin{cases} \frac{d\boldsymbol{\lambda}(t)}{dt} = -\boldsymbol{\lambda}(t)^\top \frac{\partial f(\boldsymbol{h}_t, \boldsymbol{h}_{t-\tau}, t; \boldsymbol{w})}{\partial \boldsymbol{h}_t} - \boldsymbol{\lambda}(t+\tau)^\top \frac{\partial f(\boldsymbol{h}_{t+\tau}, \boldsymbol{h}_t, t; \boldsymbol{w})}{\partial \boldsymbol{h}_t} \chi_{[0,T-\tau]}(t),\ t <= T \\ \boldsymbol{\lambda}(T) = \frac{\partial L(\boldsymbol{h}(T))}{\partial \boldsymbol{h}(T)}, \end{cases} \tag{2}$$

where $\chi_{[0,T-\tau]}(\cdot)$ *is a typical characteristic function.*

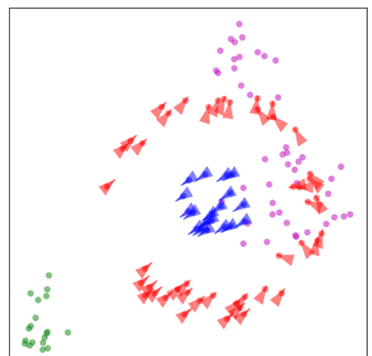
$$\frac{dL}{d\boldsymbol{w}} = \int_T^0 -\boldsymbol{\lambda}(t)^\top \frac{\partial f(\boldsymbol{h}_t, \boldsymbol{h}_{t-\tau}, t; \boldsymbol{w})}{\partial \boldsymbol{w}} dt.$$

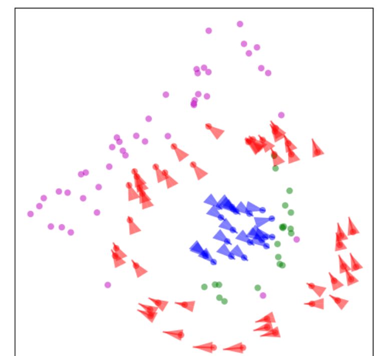
Example: ***concentric annuli***



$$\dot{x} = f(x(t-1), \theta)$$
$$t \in [0, 1]$$

$$if\ t \leq 0, x(t) = x_0$$



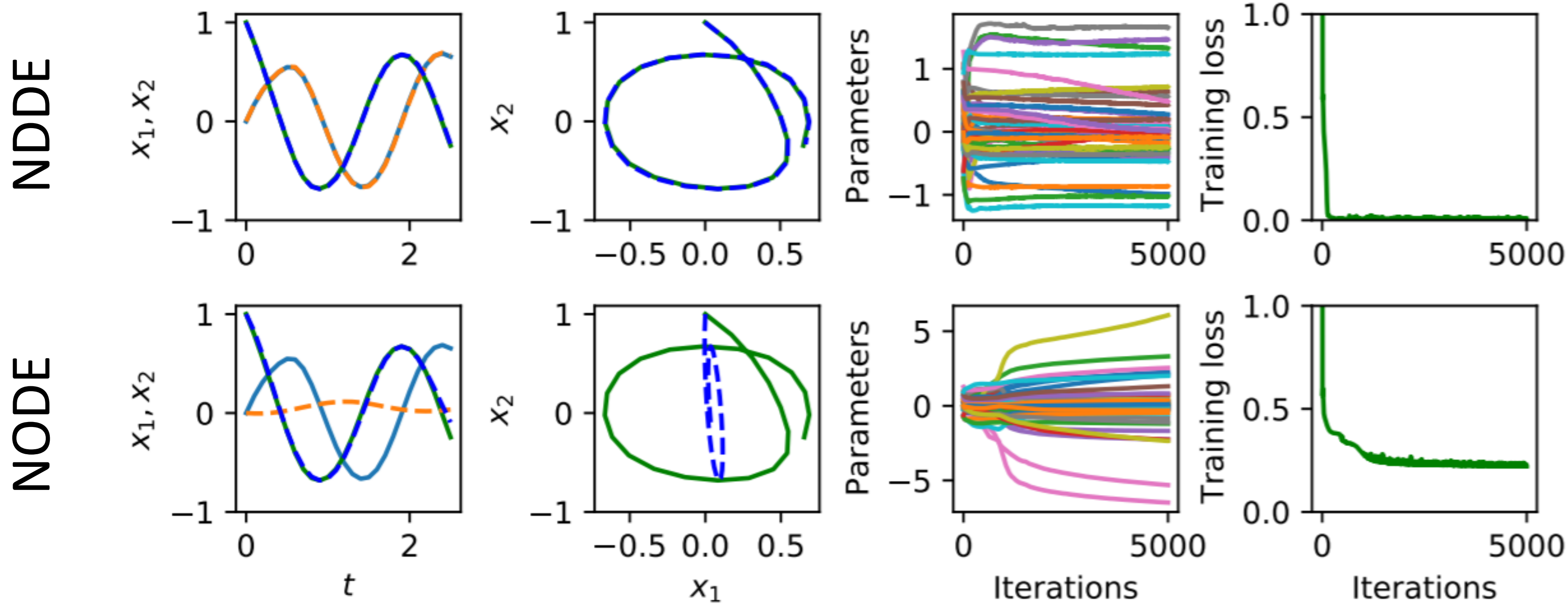


$$\dot{x} = f(x(t), \theta)$$
$$t \in [0, 1]$$

$$x(0) = x_0$$

Example: ***2-dimentional DDEs***

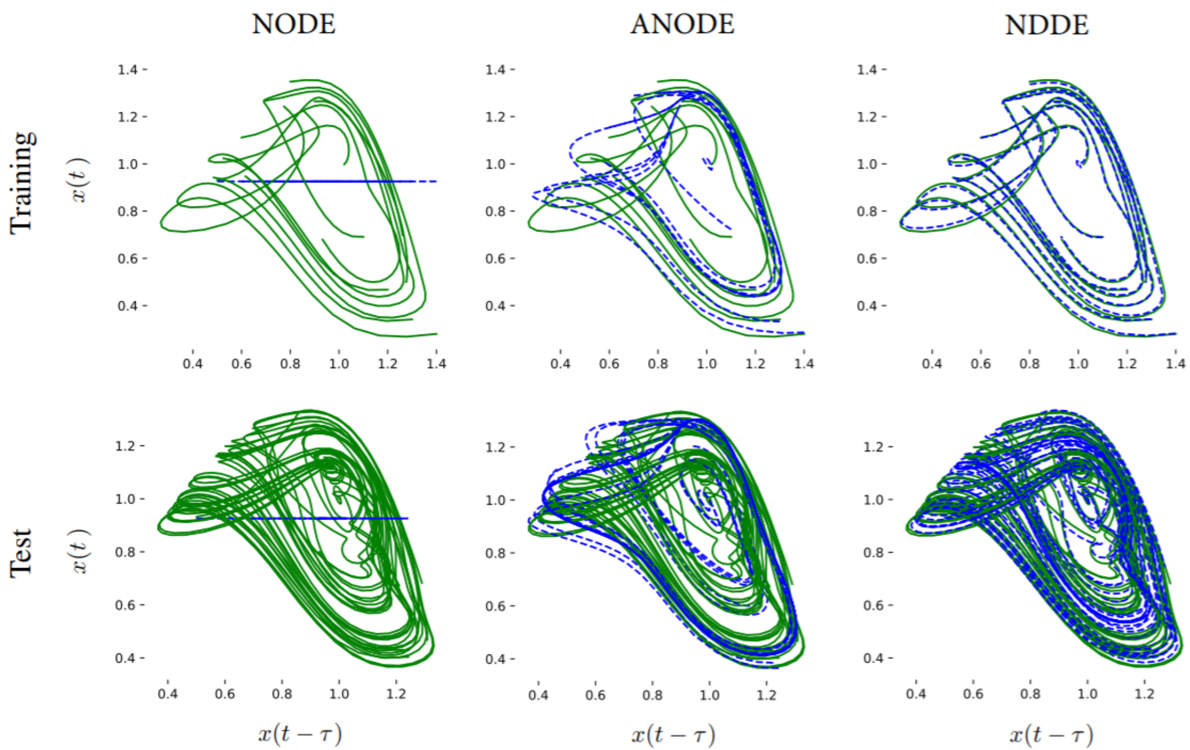
$$\dot{\boldsymbol{x}} = \boldsymbol{A}\tanh(\boldsymbol{x}(t) + \boldsymbol{x}(t-\tau)) \text{ with } \boldsymbol{x}(t) = \boldsymbol{x}_0 \text{ for } t < 0$$



Example: Mackey-Glass system

$$\dot{x} = \beta \frac{x(t-\tau)}{1+x^n(t-\tau)} - \gamma x(t)$$

- $x(t)$ is the number of the blood cells,
- β, n, τ, γ are the parameters of biological significance



Mackey, M. and Glass, L. Oscillation and chaos in physiological control systems. **Science**, 1977

Example: Image datasets

	CIFAR10	MNIST	SVHN
NODE	$53.92\% \pm 0.67$	$96.21\% \pm 0.66$	$80.66\% \pm 0.56$
NDDE	$55.69\% \pm 0.39$	$96.22\% \pm 0.55$	$81.49\% \pm 0.09$
NODE+NDDE	$\mathbf{55.89\% \pm 0.71}$	$\mathbf{97.26\% \pm 0.22}$	$\mathbf{82.60\% \pm 0.22}$
A1+NIDE	$56.14\% \pm 0.48$	$97.89\% \pm 0.14$	$81.17\% \pm 0.29$
A1+NDDE	$56.83\% \pm 0.60$	$97.83\% \pm 0.07$	$82.46\% \pm 0.28$
A1+NODE+NDDE	$\mathbf{57.31\% \pm 0.61}$	$\mathbf{98.16\% \pm 0.07}$	$\mathbf{83.02\% \pm 0.37}$
A2+NODE	$57.27\% \pm 0.46$	$98.25\% \pm 0.08$	$81.73\% \pm 0.92$
A2+NDDE	$58.13\% \pm 0.32$	$98.22\% \pm 0.04$	$82.43\% \pm 0.26$
A2+NODE+NDDE	$\mathbf{58.40\% \pm 0.31}$	$\mathbf{98.26\% \pm 0.06}$	$\mathbf{83.73\% \pm 0.72}$
A4+NODE	$58.93\% \pm 0.33$	$98.33\% \pm 0.12$	$82.72\% \pm 0.60$
A4+NDDE	$59.35\% \pm 0.48$	$98.31\% \pm 0.03$	$82.87\% \pm 0.55$
A4+NODE+NDDE	$\mathbf{59.94\% \pm 0.66}$	$\mathbf{98.52\% \pm 0.11}$	$\mathbf{83.62\% \pm 0.51}$

Table 1: The test accuracies with their standard deviations over 5 realizations on the three image datasets. In the first column, p (=1, 2, or 4) in Ap means the number of the channels of zeros into the input image during the augmentation of the image space $\mathbb{R}^{c\times h\times w} \to \mathbb{R}^{(c+p)\times h\times w}$ (Dupont et al., 2019). For each model, the initial (resp. final) time is set as 0 (resp. 1), and the delays of the NDDEs and its extensions are all set as 1, simply equal to the final time.

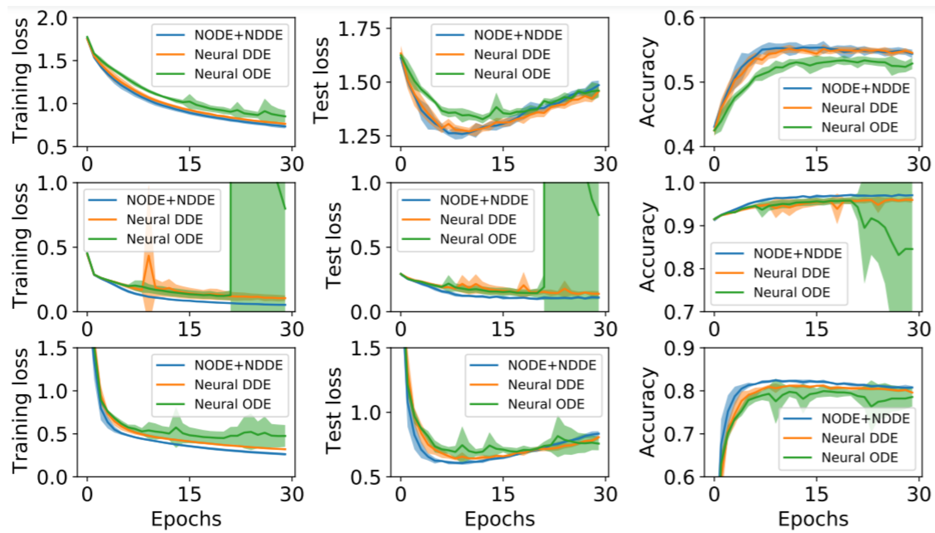


Figure 8: The training loss (left column), the test loss (middle column), and the accuracy (right column) over 5 realizations for the three image sets, i.e., CIFAR10 (top row), MNIST (middle row), and SVHN (bottom row).

Conclusion and future directions

Conclusion

NDDEs with dependency on a time delay allow to model a larger class of physical systems, in particular adding the possibility of crossing paths in phase space.

Future directions

- Applications
  - Continuous-time series modelling (Irregular-sampled, physics models)
  - Generative modelling (continuous normalizing flows)
  - Applications to traditional mathematical modelling (SIR, . . .), and traditional machine learning problems
- Differential Equations
  - Higher-Order Differential Equations
  - Stochastic Differential Equations
  - Partial differential equations
- Numerical optimization of Neural ODEs
  - Regularizing learned dynamics to be faster to solve
- And …

Thank you ！