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Unconstrained Parametrization of Dissipative and Contracting Neural Ordinary Differential Equations

Daniele Martinelli,

Clara Lucía Galimberti,

Ian R. Manchester,

Luca Furieri,

Giancarlo Ferrari-Trecate

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THE UNIVERSITY OF SYDNEY

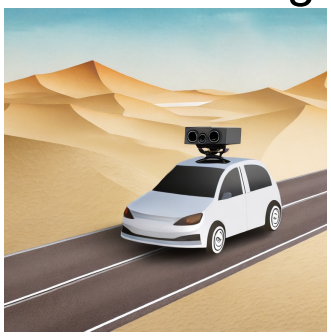
NCCR Automation

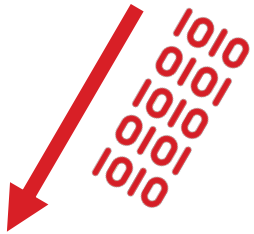
Learning for Complex Systems

Robotics

Power Grids

Autonomous Driving Vehicles

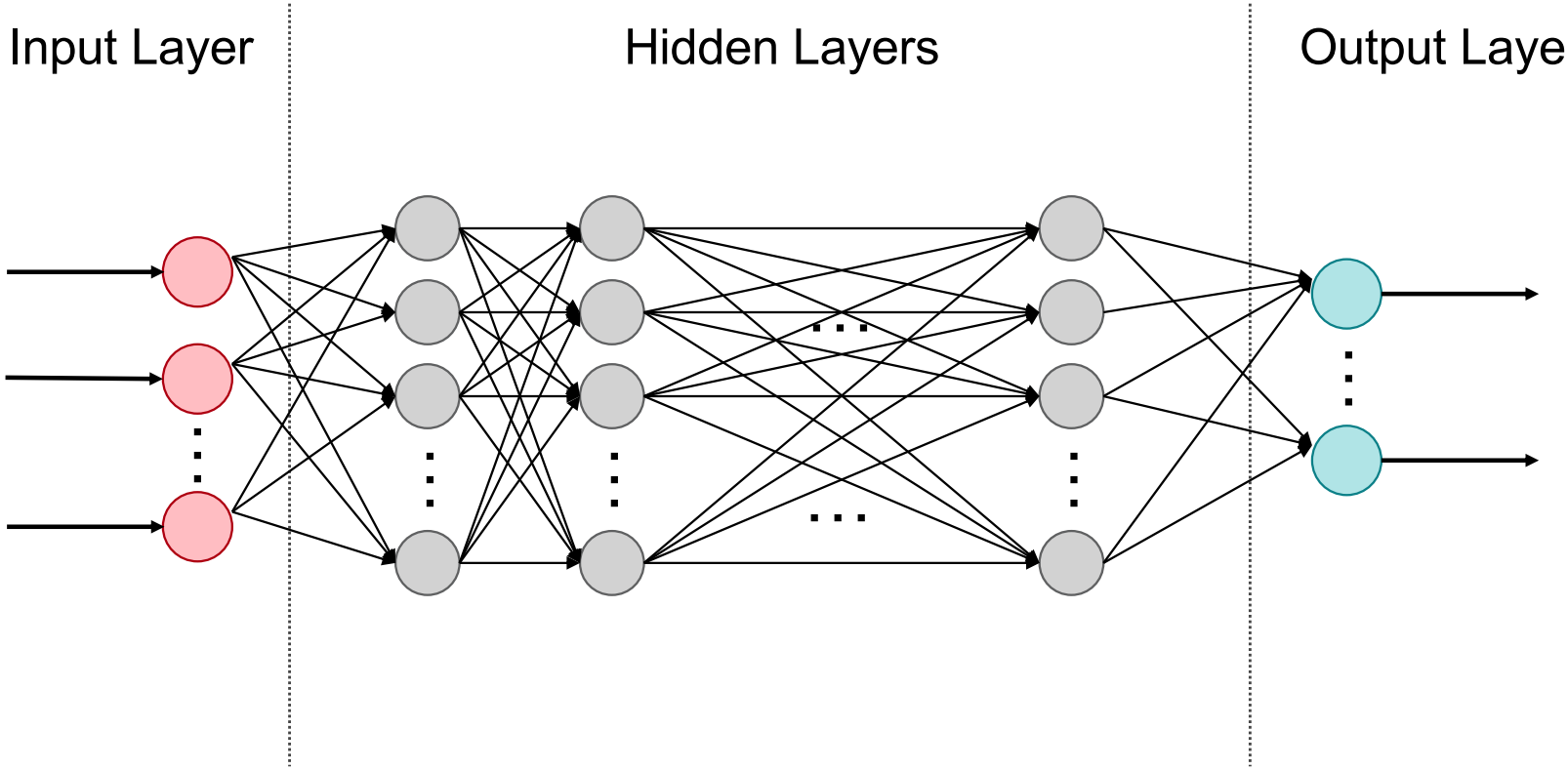




Machine Learning

Deep Neural Networks

Deep Neural Networks (DNNs)



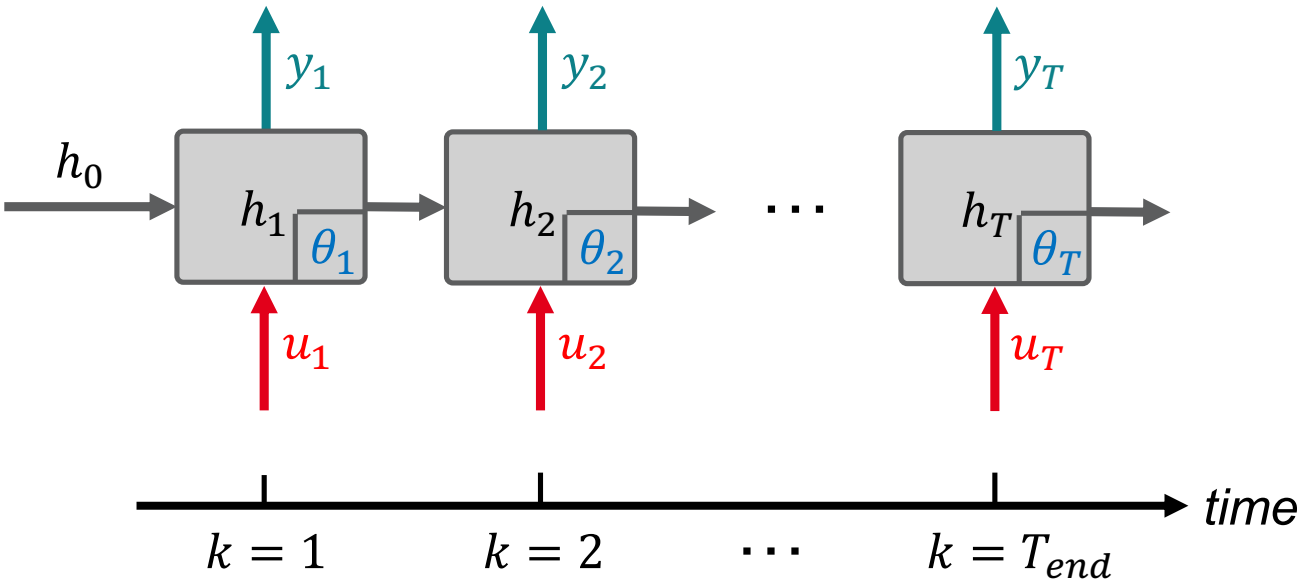
ODE-based DNNs

Ordinary Differential Equation (ODE)

$$\frac{d\,h(t)}{dt} = f(h(t), t, \theta(t), u(t))$$
$$h(0) = h_0$$

Discretization

$$h_{k+1} = h_k + f(h_k, \theta_k, u_k),\ k \in \{0 \dots T_{end}\}$$



Can be seen as a DNN!

u_k: Inputs
y_k: Outputs
h_k: States
θ_k: Parameters

Neural-ODEs

Neural Ordinary Differential Equations

Ricky T. Q. Chen*, Yulia Rubanova*, Jesse Bettencourt*, David Duvenaud
University of Toronto, Vector Institute
{rtqichen, rubanova, jessebett, duvenaud}@cs.toronto.edu

- Continuous time system
- Use of modern ODE solvers for the evolution of the model
- Integration methods with
  - Fixed-steps
  - Variable-steps
- Open-Source library

Drawbacks for system identification & control:

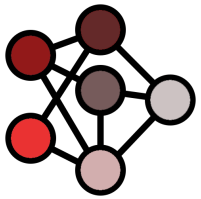
- No guarantees
  - Sensitive to perturbations in I/O
  - No Stability guarantees

Contributions & Contents

Goal: Design class of NeuralODE that enjoys stability properties by design

Targeted Properties

Stability notions



NodeRENs

Guaranteed properties through
Unconstrained Parametrization

Numerical Example

Nonlinear System Identification

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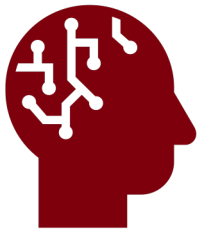
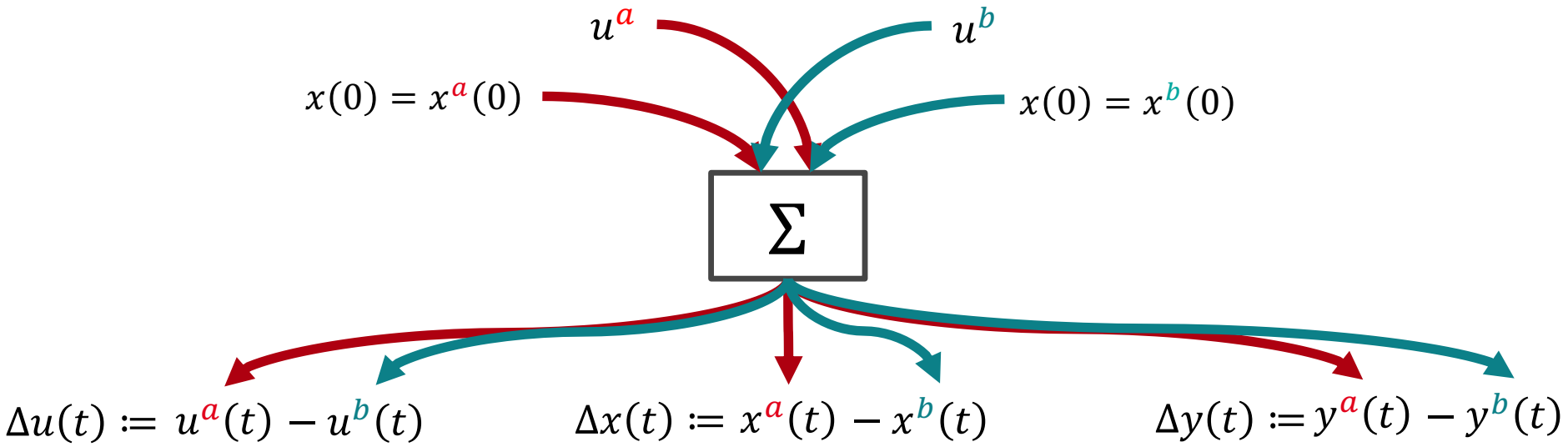
Targeted Properties



Incremental Properties

MIMO system $\Sigma = \begin{cases} \dot{x}(t) = f(x(t), u(t)) \\ y(t) = g(x(t), u(t)) \end{cases}$

Comparison of different trajectories

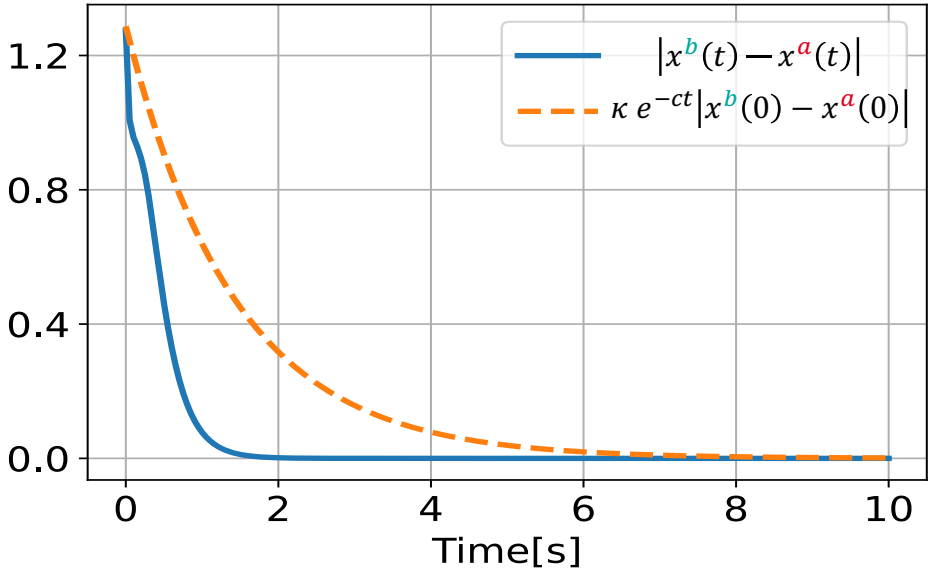


Contractivity

Definition

The system Σ is contracting if for any $x^a(0),\ x^b(0)$ and $u^a = u^b$:

$$\left|x^b(t) - x^a(t)\right| \leq \kappa\, e^{-ct}\left|x^b(0) - x^a(0)\right| \qquad \forall t \geq 0 \qquad \kappa, c > 0$$



If the system has an equilibrium point:

Contractivity

↓

(Globally) Exponential Stability!

Dissipativity

Internal energy → Storage function: $V(\cdot)$

Exchange through inputs/outputs → supply rate: $s(\cdot,\cdot)$

Definition

The system Σ is dissipative w.r.t. a supply rate $s(\cdot,\cdot)$, if there exists a storage function $V(\cdot)$ such that:

$$V\big(x(t_1)\big) - V\big(x(t_0)\big) \leq \int_{t_0}^{t_1} s\big(u(t), y(t)\big)dt \ , \qquad \forall t_1 \geq t_0$$

Why dissipativity?

- Tight connection with *Lyapunov stability* *(under mild conditions)*

Common choices of supply rate $s(\cdot,\cdot)$?

Quadratic Supply Rates

$$s\big(\Delta u(t), \Delta y(t)\big) = \begin{bmatrix}\Delta y(t)\\ \Delta u(t)\end{bmatrix}^{\mathsf{T}} \begin{bmatrix}Q & S^{\mathsf{T}}\\ S & R\end{bmatrix} \begin{bmatrix}\Delta y(t)\\ \Delta u(t)\end{bmatrix}$$

Common choices of (Q, S, R):

ℓ_2 Lipschitz bound:

$\|\Delta y(t)\|_T \leq \gamma \|\Delta u(t)\|_T$ → $Q = -\frac{1}{\gamma} I, \quad R = \gamma I, \quad S = 0$

Incremental Input Passive:

$s = \Delta u(t)^{\mathsf{T}} \Delta y(t) - \nu \|\Delta u(t)\|^2$ → $Q = 0, \quad R = -2\nu I, \quad S = I$

Incremental Output Passive:

$s = \Delta u(t)^{\mathsf{T}} \Delta y(t) - \rho \|\Delta y(t)\|^2$ → $Q = -2\rho I, \quad R = 0, \quad S = I$

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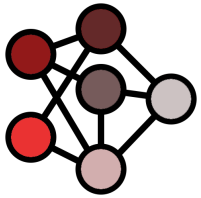
NODE-RENs



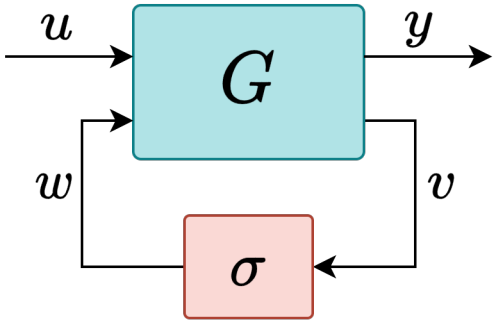
Neural ODE Recurrent Equilibrium Networks (NodeRENs)

Recurrent Equilibrium Networks: Flexible Dynamic Models with Guaranteed Stability and Robustness

Max Revay*, Ruigang Wang*, Ian R. Manchester

Continuous-Time settings + REN (Discrete-Time) = **NodeREN**

NodeREN Model:



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Linear part:

$$\begin{bmatrix} \dot{x}_t \\ v_t \\ y_t \end{bmatrix} = \begin{bmatrix} A & B_1 & B_2 \\ C_1 & D_{11} & D_{12} \\ C_2 & D_{21} & D_{22} \end{bmatrix} \begin{bmatrix} x_t \\ w_t \\ u_t \end{bmatrix} + \begin{bmatrix} b_x \\ b_v \\ b_y \end{bmatrix}$$

Nonlinear part:

$$w_t = \sigma(v_t)$$

Contracting & Dissipative NodeRENs

Theorem 1 (*Contracting NodeREN*).
A NodeREN is contracting if there exists a $P \succ 0$ and a $\Lambda \in \mathbb{D}_+$ such that:

$$\begin{bmatrix} -A^\top P - PA & -C_1^\top \Lambda - PB_1 \\ -\Lambda C_1 - B_1^\top P & W \end{bmatrix} \succ 0$$

$$\textit{with: } W = 2\Lambda - \Lambda D_{11} - D_{11}^\top \Lambda$$

Theorem 2 (*Dissipative NodeREN*).
A NodeREN is incrementally dissipative w.r.t. quadratic supply rate if there exists a $P \succ 0$ and a $\Lambda \in \mathbb{D}_+$ such that:

$$\begin{bmatrix} -A^\top P - PA & -C_1^\top \Lambda - PB_1 & -PB_2 + C_2^\top S^\top \\ -\Lambda C_1 - B_1^\top P & W & D_{21}^\top S^\top - \Lambda D_{12} \\ -B_2^\top P + SC_2 & SD_{21} - D_{21}^\top \Lambda & R + SD_{22} + D_{22}^\top S^\top \end{bmatrix} + \begin{bmatrix} C_2^\top \\ D_{21}^\top \\ D_{22}^\top \end{bmatrix} Q \begin{bmatrix} C_2^\top \\ D_{21}^\top \\ D_{22}^\top \end{bmatrix}^\top \succ 0$$

Computationally Expensive!

Can we remove constraints?

Unconstrained Parametrization

Contractivity matrix inequality

$$\begin{bmatrix} -A^\top P - PA & -C_1^\top \Lambda - PB_1 \\ -\Lambda C_1 - B_1^\top P & W \end{bmatrix} \succ 0$$

NodeREN Model:

$$\begin{bmatrix} \dot{x}_t \\ v_t \\ y_t \end{bmatrix} = \begin{bmatrix} A & B_1 & B_2 \\ C_1 & D_{11} & D_{12} \\ C_2 & D_{21} & D_{22} \end{bmatrix} \begin{bmatrix} x_t \\ w_t \\ u_t \end{bmatrix} + \begin{bmatrix} b_x \\ b_v \\ b_y \end{bmatrix}$$

$$w_t = \sigma(v_t)$$

$$H = X^\top X + \epsilon I \succ 0 \text{ always!}$$

$$P = X_P^\top X_P + \epsilon_P I \succ 0$$

How we obtain a C-NodeREN

I) Choose freely X, X_p, build H, P II) Get matrices from H, P III) Choose freely the remaining ones

Enforcing Dissipativity follows similar steps!

$H = X^\top$ …
$P = X_P^\top X_P + \epsilon_P I$

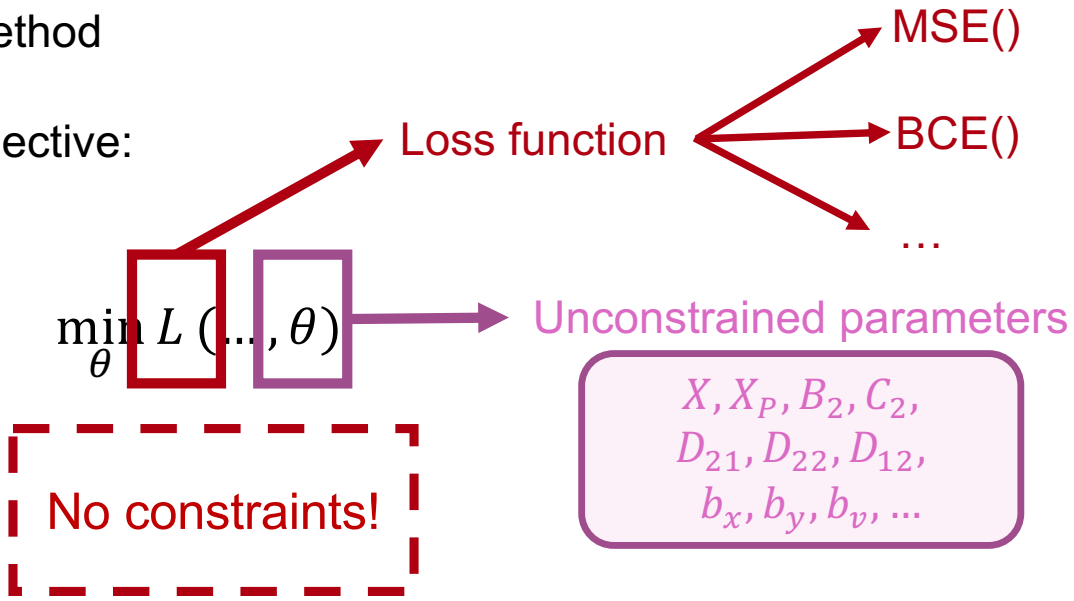
$A, B_1,$
C_1, D_{11}, Λ

$D_{12},$
$D_{21}, D_{22},$
$b_x, b_y, b_v, \ldots$

Unconstrained Parameters

How To Train NodeRENs

- Choose the property to be guaranteed: contractivity and/or incremental dissipativity
- Choose an integration method
- Define a minimization objective:



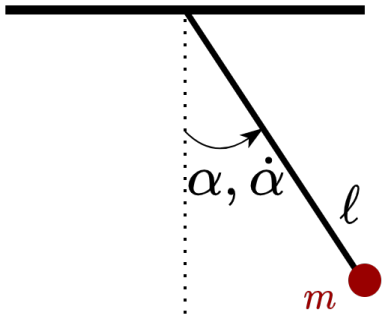
- Easy to optimize over with gradient descent or stochastic variants (e.g., SGD, ADAM)

PyTorch

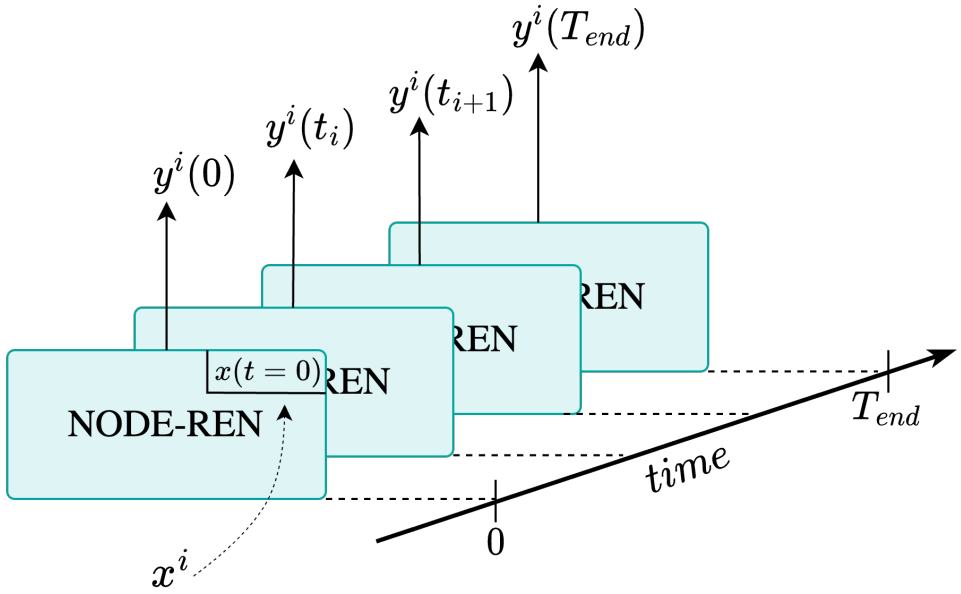
Numerical Example

System Identification (SYSID)

- **System:** Pendulum

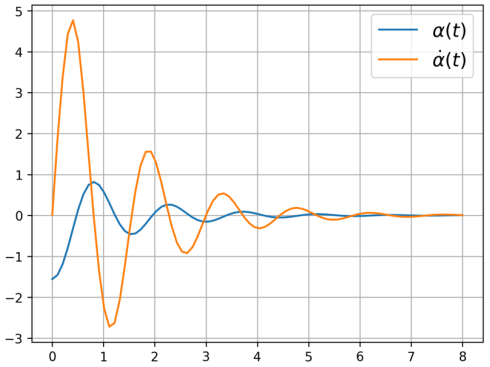


$$\ell\ddot{\alpha}(t) + \beta\dot{\alpha}(t) + g\sin\alpha(t) = 0$$



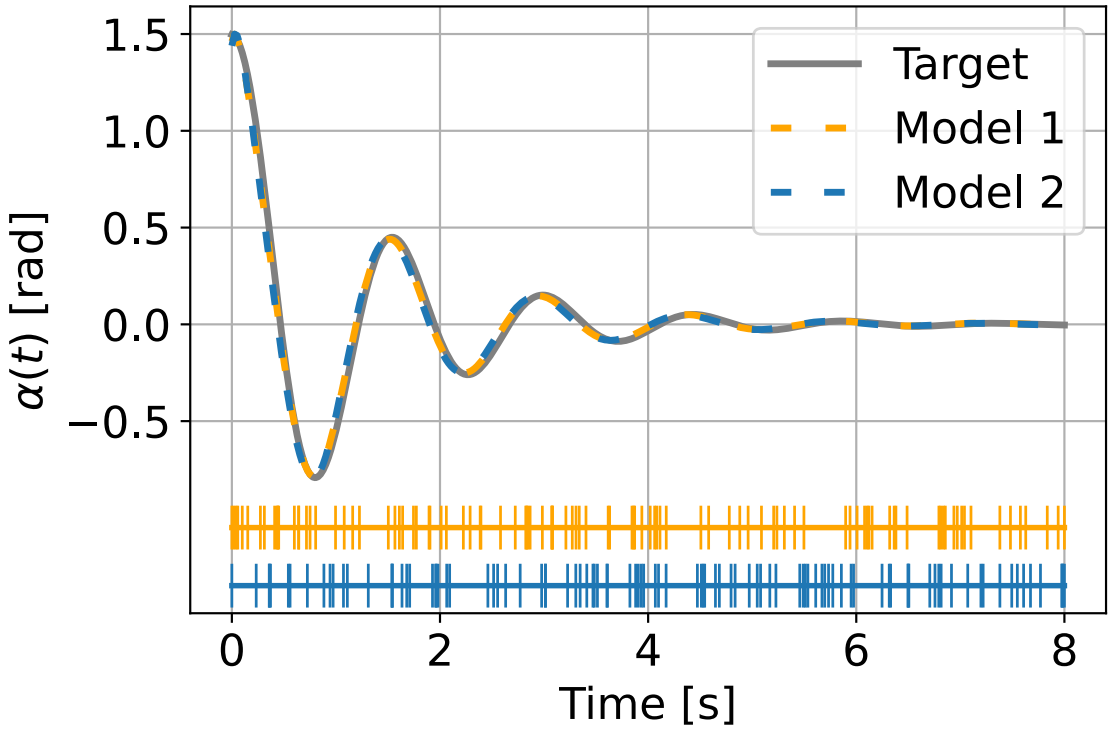
- **Loss Function:** Mean Squared Error (MSE)

- **Experiments:** $\begin{bmatrix}\alpha(0)\\ \dot{\alpha}(0)\end{bmatrix}$ →

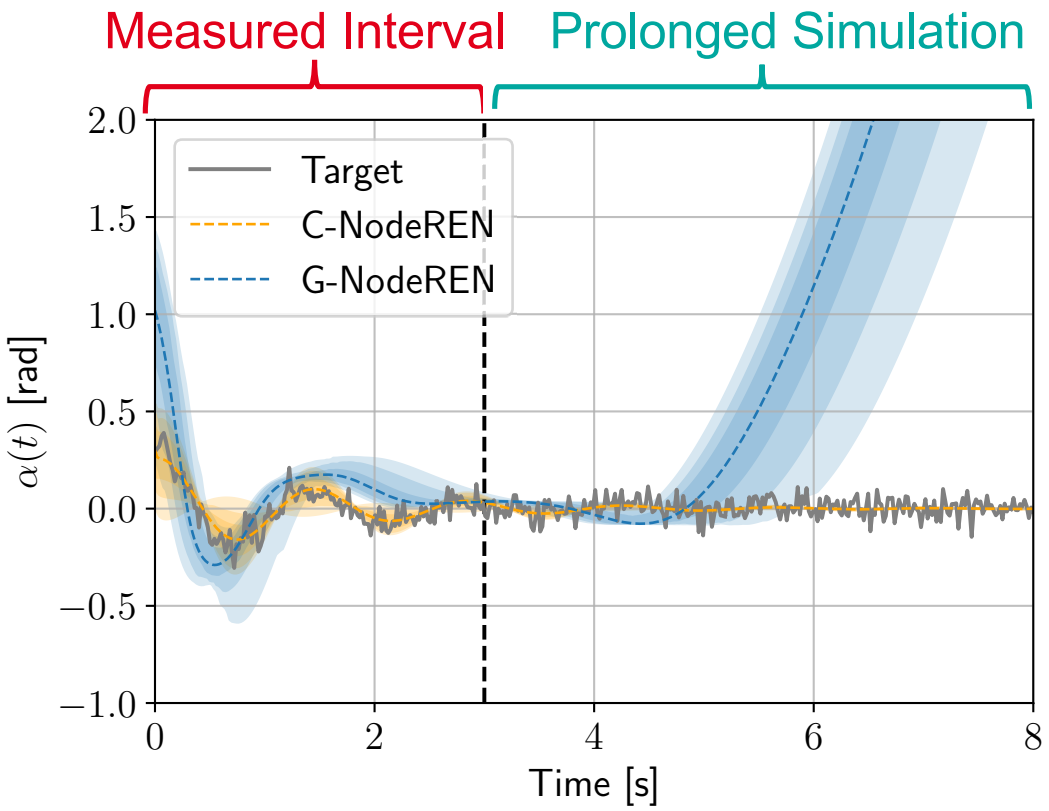


SYSID - Irregularly Sampled Data

Can handle naturally irregularly sampled data! (e.g., from sensor networks)



SYSID – Why Enforcing Contractivity



- We enforce contractivity by design
  ↪ Embedding prior knowledge
- Can be simulated for longer time horizons (w.r.t. training time)
- Improved numerical stability during simulations

Conclusions

Summary

- Class of DNN with guarantees of contractivity and/or inc. dissipativity by design
- Nonlinear system identification embedding contractivity/inc. dissipativity priors

Future Developments

- Beyond SYSID Applications:
  - Optimal control
  - Classification tasks (ML)
- Real-world applications
- Incorporating integration schemes preserving contractivity

Thank you!

Paper

How To Train NodeRENs

COME FACCIO IL TRAINING effettivamente (BACKUP ALLA FINE)

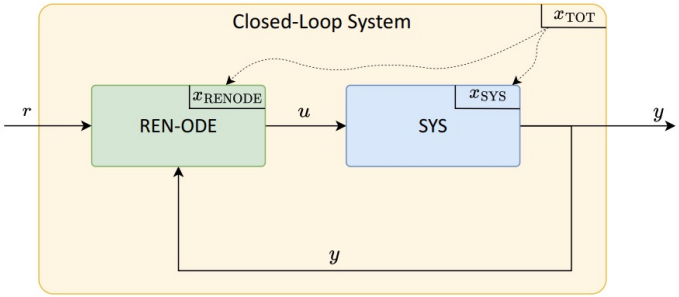


Figure 3.2: Scheme of the implementation of a feedback closed-loop system using Torchdiffeq library. The reference signal r must be defined a priori or generated by a "signal generator" inside the closed-loop system.

Algorithm 3.2 Pseudo-code of the Feed-Forward function in a Closed-Loop system.

Input: model (total system), time instant t, state of the total system $x_{TOT}(t)$.

$x_{\text{RENODE}},\ x_{\text{SYS}} = \text{split}(x_{\text{TOT}}(t))$ ▷ Split state vector in two.

$y(t) = \text{SYS.output}(t, x_{\text{SYS}})$ ▷ output evaluation of SYS

$\dot{x}_{\text{REN-ODE}}(t) = \text{RENODE.forward}(t, x_{\text{SYS}})$ ▷ state evolution of RENODE

$u_{\text{RENODE}}(t) = \text{RENODE.output}(t, x_{\text{SYS}})$ ▷ output evaluation of RENODE

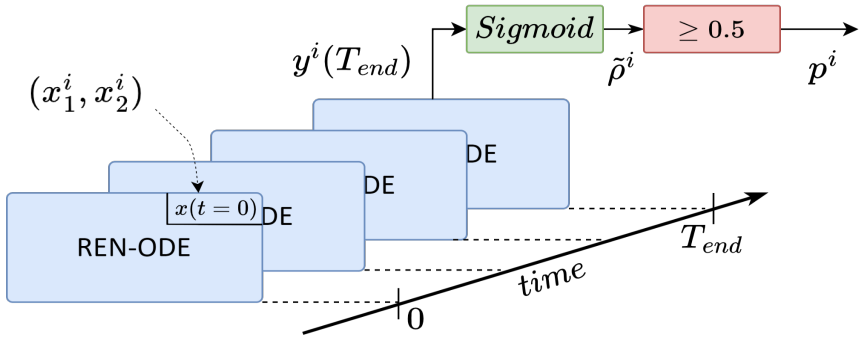
$\dot{x}_{\text{SYS}}(t) = \text{SYS.forward}(t, x_{\text{SYS}}, u_{\text{RENODE}}(t))$ ▷ state evolution of SYS

return $[\dot{x}_{RENODE}\ ,\ \dot{x}_{SYS}]$ ▷ Return the derivative of both states

Binary Classification

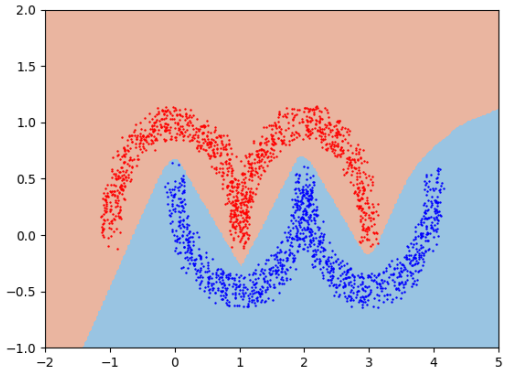
Classification Problem:

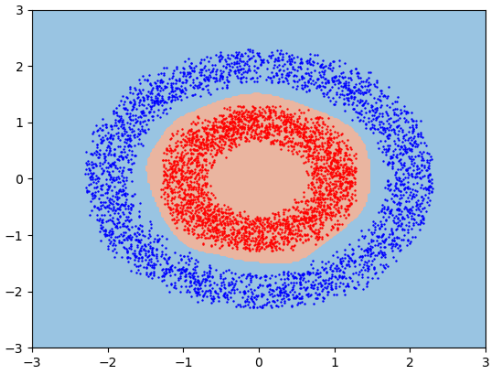
- **Input**: 2 features
- **Label**: binary { 0, 1 }

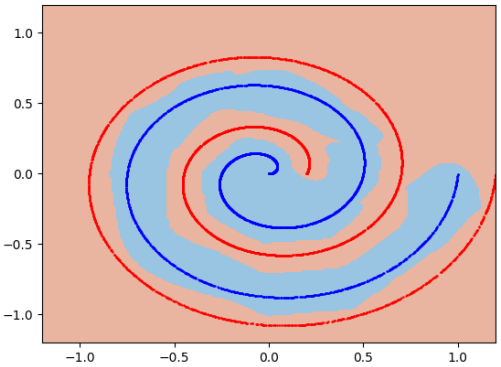


Loss Function:
Binary Classification Entropy (BCE):

$$\ell(\tilde{p}, \hat{y}) = -(\hat{y}\log(\tilde{p}) + (1-\hat{y})\log(1-\tilde{p}))$$

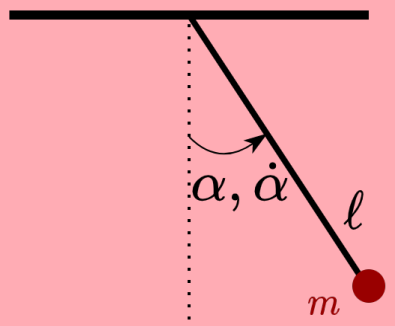




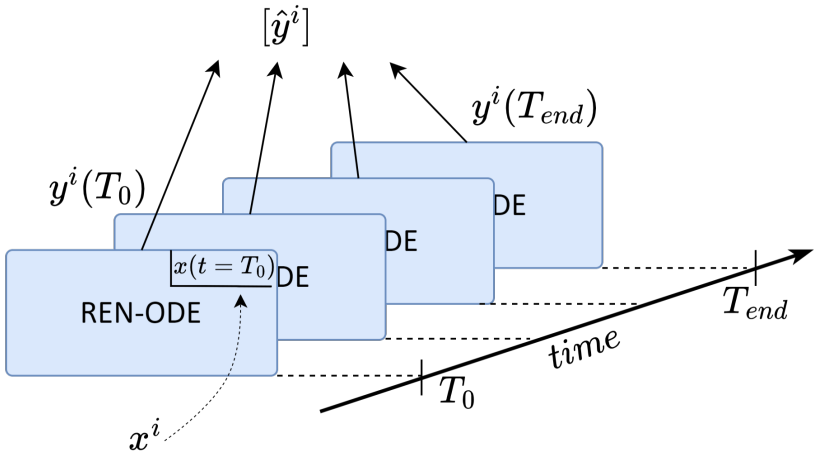


System Identification (SYSID)

Nonlinear Pendulum:



$$\ell\ddot{\alpha}(t) + \beta\dot{\alpha}(t) + g\sin\alpha(t) = 0$$

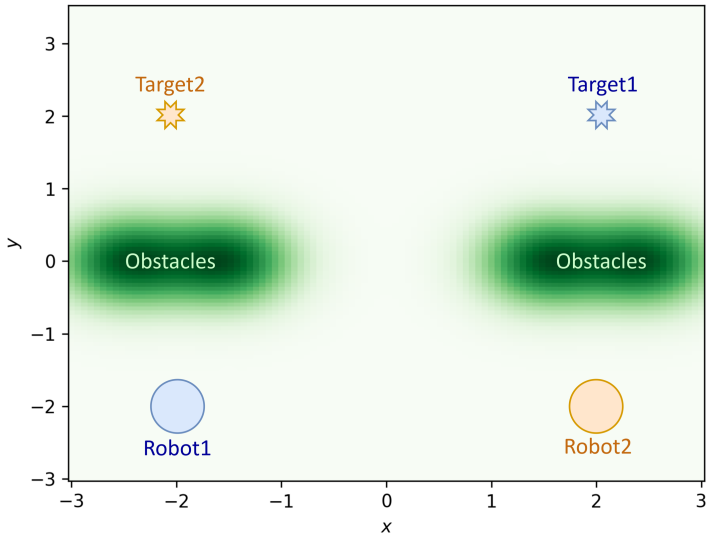


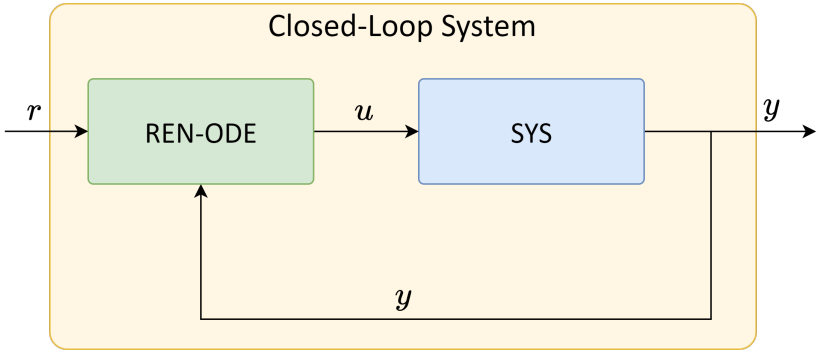
Loss Function:

Mean Squared Error (MSE):

$$L(y,\hat{y}) = MSE(y,\hat{y}) = \frac{1}{\eta}\sum_{i=0}^{\eta}\sum_{t=T_0}^{T_{end}}\left\|y^i(t) - \hat{y}^i(t)\right\|^2$$

Optimal Control





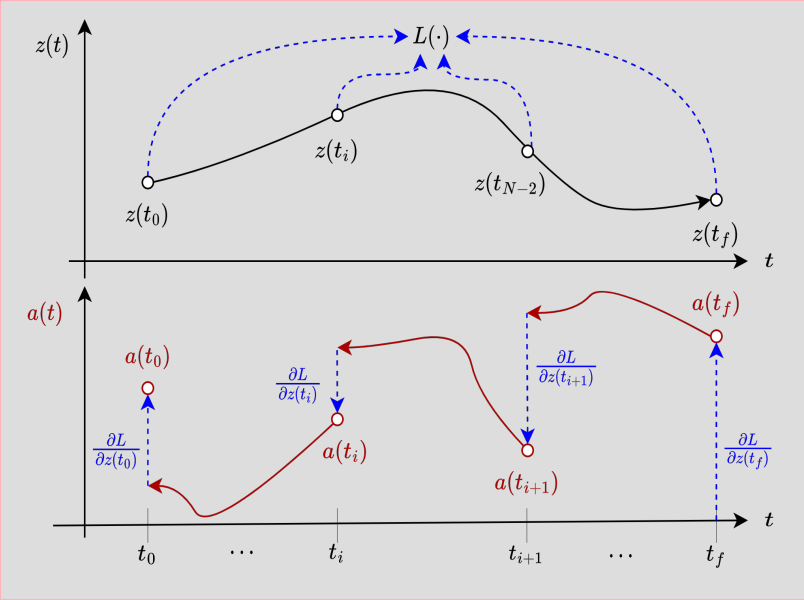
Optimal Control Policy (loss function):

$$L = \sum_{k=0}^{T_{end}/T_s} l_{traj}(x_{t_k}, u_{t_k}) + l_{ca}(x_{t_k}) + l_{obst}(x_{t_k})$$

Neural-ODE

Training Phase

- Gradient are computed by solving another ODE from $T_{end} \rightarrow t_0$.
- Don't backpropagate through the operations of the solver.
- No need to store activations, O(1) memory gradient



$$a(t) = \frac{\partial L}{\partial z(t)} \longrightarrow \frac{d}{dt}a(t) = -a(t)^{\mathsf{T}} \frac{\partial f(z(t), t, \theta)}{\partial z}$$

Assumptions

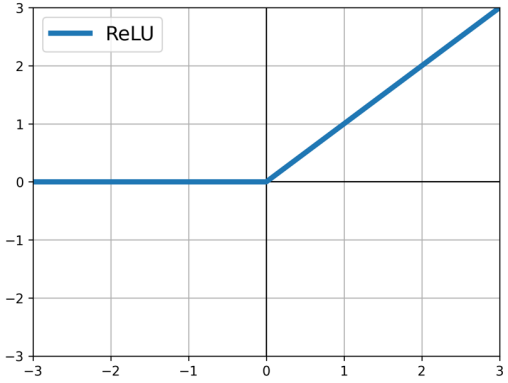
Assumption on activation function $\sigma(\cdot)$:

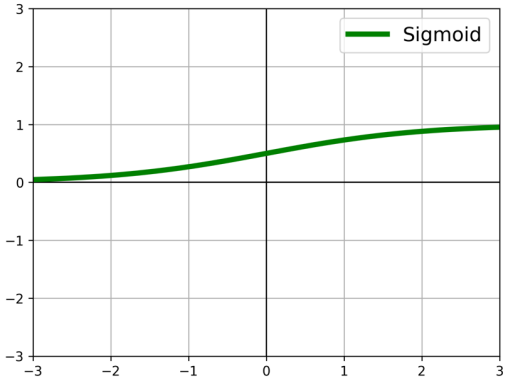
$$0 \leq \frac{\sigma(y)-\sigma(x)}{y-x} \leq 1$$

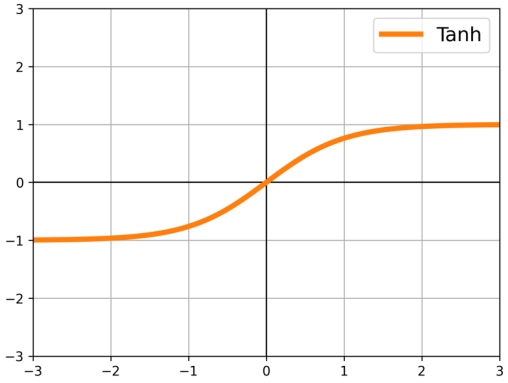
Conic Combination

$$\Gamma_t = \begin{bmatrix} \Delta v_t \\ \Delta w_t \end{bmatrix}^{\top} \begin{bmatrix} 0 & \Lambda \\ \Lambda & -2\Lambda \end{bmatrix} \begin{bmatrix} \Delta v_t \\ \Delta w_t \end{bmatrix} \geq 0,$$

Popular activation functions satisfy it already! (e.g., $ReLU(\cdot), Sigmoid(\cdot), \tanh(\cdot)$ ✓)







Dissipative Direct Parametrization

Dissipativity matrix inequality

$$\begin{bmatrix} -A^\top P - PA & -C_1^\top \Lambda - PB_1 & -PB_2 + C_2^\top S^\top \\ -\Lambda C_1 - B_1^\top P & W & D_{21}^\top S^\top - \Lambda D_{12} \\ -B_2^\top P + SC_2 & SD_{21} - D_{21}^\top \Lambda & R + SD_{22} + D_{22}^\top S^\top \end{bmatrix} + \begin{bmatrix} C_2^\top \\ D_{21}^\top \\ D_{22}^\top \end{bmatrix} Q \begin{bmatrix} C_2^\top \\ D_{21}^\top \\ D_{22}^\top \end{bmatrix}^\top \begin{matrix} Q < 0 \\ > 0 \end{matrix}$$

$$H = \begin{bmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{bmatrix} = X^\top X + \epsilon I \quad > 0 \text{ always!}$$

How we obtain from H a RNodeREN?

I) Pick free parameters

$X, \cancel{B_2}, C_2, \cancel{D_{12}}, \cancel{D_{21}}, \cancel{D_{22}}, b_x, b_y, b_v, \ldots$

II) Build matrix H

$H = X^\top X + \epsilon I$

III) Retrieve remaining matrices using H

$A, B_1, B_2, C_1, D_{11}, D_{12}, D_{22}$