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nnodely

A FRAMEWORK FOR DESIGN MODEL-STRUCTURED NEURAL NETWORKS FOR MODEL AND CONTROL PHYSICAL SYSTEMS

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Overview

The Neu4mes Project

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Pricipal Investigator Gastone P. Rosati P., University of Trento

Founded by the **Italian Ministry of University and Research** (MUR) under the *Science Italian Found 2023* program, for **1.2 Million Euros**.

Aim Develop a new approach to model and control physical system using **Model-Structured Neural Networks**

Outcome the nnodely framework, a **wiki website** for collecting MSNN models.

Case Study Several autonomous systems, including: **Drones**, **Quadrupeds**, **Vehicles**.

More details at https://tonegas.it/

Motivation

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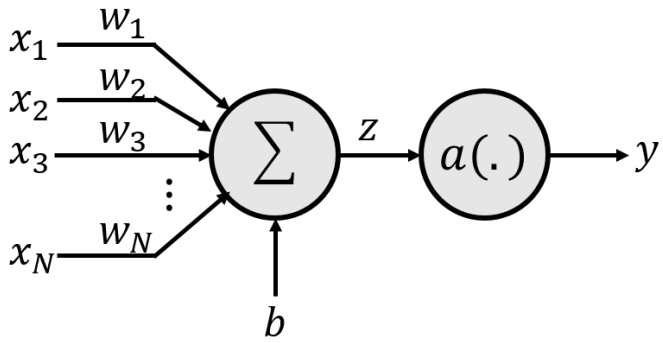
Why Model-Structured Neural Networks?

The Perceptron

- A **neural network** (NN) is a mathematical model inspired by the structure of the human brain
- The basic component of a NN is the ***Perceptron***[1]

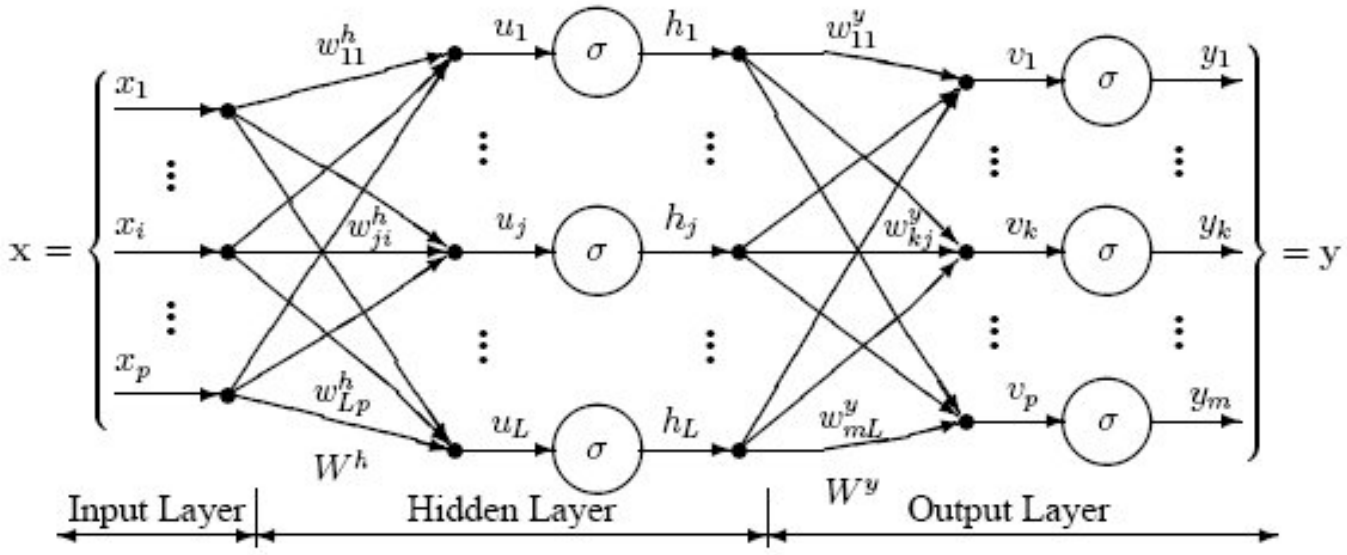


- From a mathematical point of view:

$$z = \bar{w}^T \bar{x} + b, \quad y = a(z)$$

[1]Frank Rosenblatt. "The perceptron: a probabilistic model for information storage and organization in the brain.". In: *Psychological review* (1958).

From Single- to Multi-layer Perceptron



- Multiple perceptrons can be concatenated to model general nonlinear functions (see Tensorflow Playground)
- **Universal approximation theorem**: a NN with a single hidden layer can approximate any continuous function[2]

[2]George Cybenko. "Approximation by superpositions of a sigmoidal function". In: *Math. Control Signal Systems* (1989).

The NN Internal Structure Matters

- *Computer vision*: **convolutional neural networks**, embedding the concept of spatial invariant[3]

[3] Yann LeCun, Koray Kavukcuoglu, and Clement Farabet. "Convolutional networks and applications in vision". In: *Proceedings of 2010 IEEE International Symposium on Circuits and Systems*. 2010.

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- *Natural language processing*: **transformers** embed the concept of self-attention[6] (example: chatGPT)

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Data-driven approach

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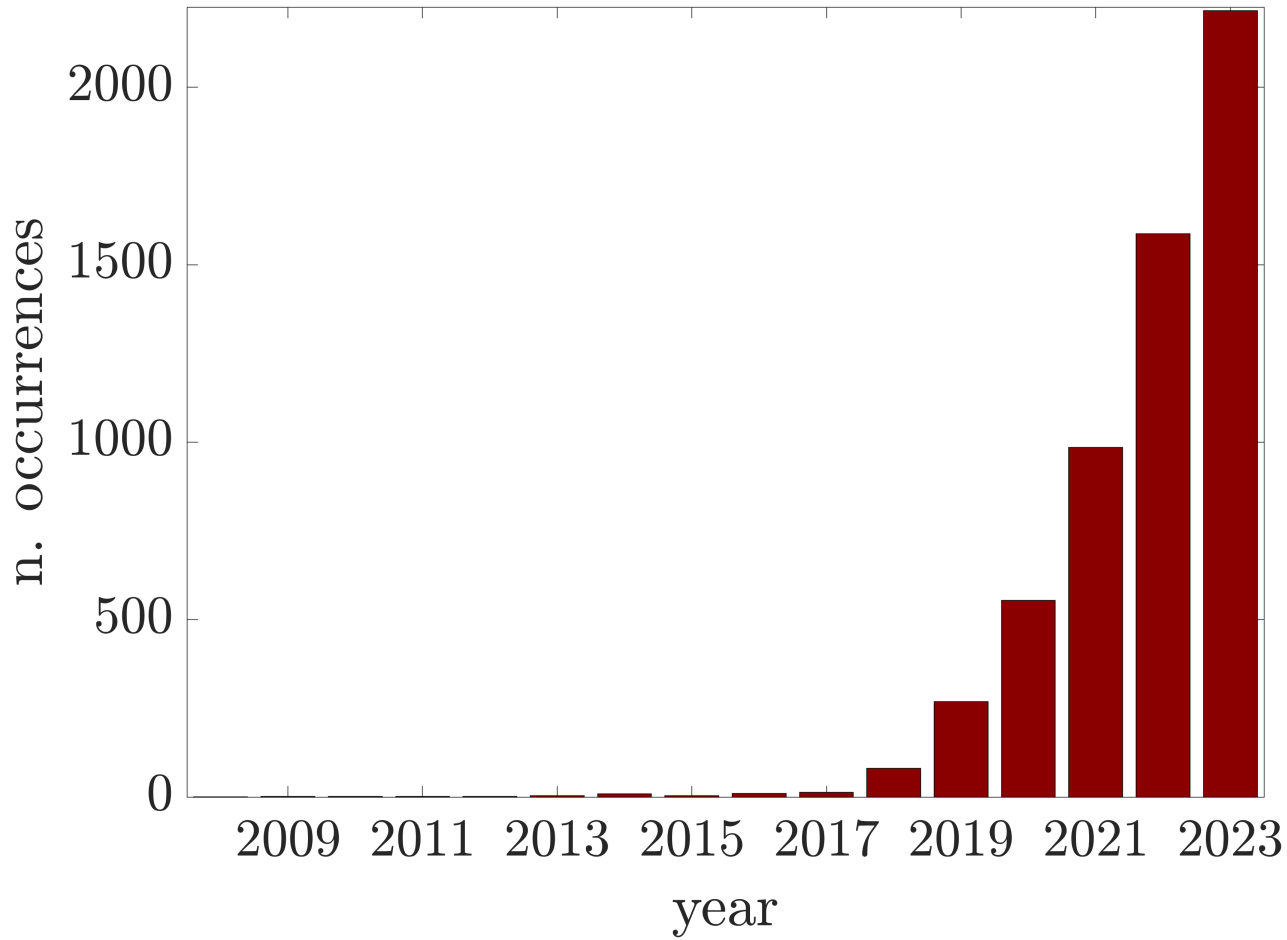
Model-Structured Neural Networks (MS-NN)

- **Flexibility** of data-driven (NN) techniques
- Embed **domain-specific knowledge** into the NN's internal **structure** $\longrightarrow$ increased **explainability** + **generalization**

Motivation

Related Work

Emerging Interest in Explainable AI



Keywords *"interpretable machine learning"*, *"explainable machine learning"* and *"explainable neural networks"* in Scopus

Overview of Physics-Driven NN Approaches

How to embed physics- or model-based knowledge in NNs?

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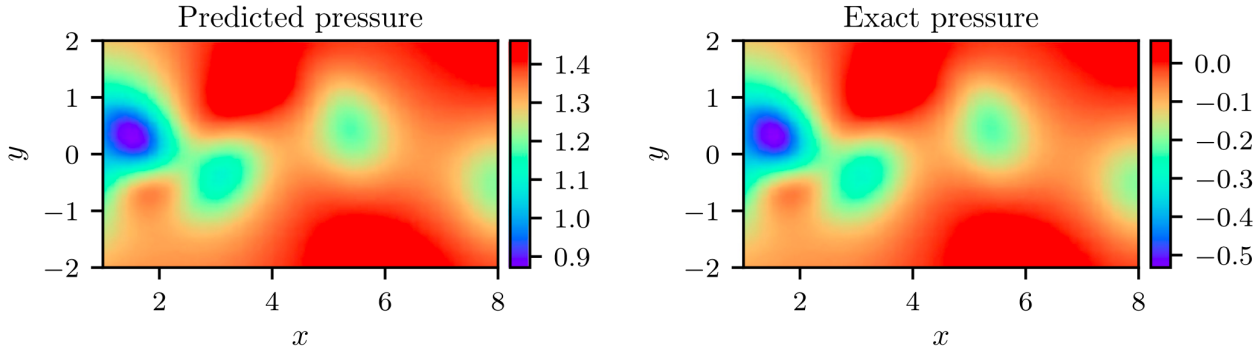
- **Design a loss function** for the NN training, e.g. to conserve energy or satisfy a PDE
- **Design of optimization algorithms**

Physics-informed NNs (PINNs), Raissi et at. (2019)

- **Idea**: Data-driven solution or discovery of complex PDEs
- **How**: *Structured loss function* based on the PDE residuals, but using deep *unstructured* NNs
- **Pros**: Learn the solution of PDEs using small training datasets; accelerate simulations of complex systems
- **Examples**: Fluid dynamics (Navier Stokes), quantum mechanics, solid mechanics, reaction-diffusion[7]. **Note**: no modeling of real physical systems, only PDEs



[7] M. Raissi, P. Perdikaris, and G.E. Karniadakis. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations". In: *Journal of Computational Physics* (2019).

Other approaches related to PINNs

- **Hamiltonian**[8] and **Lagrangian NNs**[9] that learn to conserve energy in mechanical systems and robotic tasks
- **Pontryagin AI**[10] to learn the policies of optimal control tracking problems (OCPs):
  - NN to approximate the controls of an OCP
  - NN trained with a tracking loss function
  - No need to solve the adjoint equations of the OCP
- NNs to approximate the value function of Hamilton-Jacobi-Bellman equations for **dynamic programming**[11]

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[8] Sam Greydanus, Misko Dzamba, and Jason Yosinski. *Hamiltonian Neural Networks*. 2019.

[9] Michael Lutter, Kim Listmann, and Jan Peters. "Deep Lagrangian Networks for end-to-end learning of energy-based control for under-actuated systems". In: 2019.

[10] Lucas Böttcher, Nino Antulov-Fantulin, and Thomas Asikis. "AI Pontryagin or how artificial neural networks learn to control dynamical systems". In: *Nature Communications* (2022).

[11] Murad Abu-Khalaf and Frank L. Lewis. "Nearly optimal control laws for nonlinear systems with saturating actuators using a neural network HJB approach". In: *Automatica* (2005).

Combining NNs and analytical models

- **Idea**: Use NNs to improve the prediction of analytical models
- **How**: Augment an analytical model with NNs to better learn some complex dynamics
- **Pros**: No need to learn the entire model from scratch; partly preserve the physical meaning of the model
- **Examples**:
  - NN to learn the parameters of multibody vehicle models[12]
  - Neural tire models in multibody vehicle models[13][14]
  - Neural ODE to predict the heart rate during workouts[15]

[12] John Chrosniak, Jingyun Ning, and Madhur Behl. "Deep Dynamics: Vehicle Dynamics Modeling With a Physics-Constrained Neural Network for Autonomous Racing". In: *IEEE Robotics and Automation Letters* 9.6 (2024).

[13] Jan Węgrzynowski et al. *Learning dynamics models for velocity estimation in autonomous racing*. 2024.

[14] Taekyung Kim, Hojin Lee, and Wonsuk Lee. "Physics Embedded Neural Network Vehicle Model and Applications in Risk-Aware Autonomous Driving Using Latent Features". In: *2022 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*. 2022.

[15] Achille Nazaret et al. "Modeling personalized heart rate response to exercise and environmental factors with wearables data". In: *npj Digital Medicine* 6 (Nov. 2023).

Our Model-Structured NNs

- **Idea**: Embed domain-specific prior knowledge into the NN's internal structure
- **How**: Neuralize the structure of a physics-based model
- **Pros**: Model interpretability; improved generalization
- **Examples**: Modeling *physical systems* (unknown dyna./param.)
  - Model and control the long.-lat. vehicle dynamics[16][17]
  - Vehicle state estimation[18]
  - Model mechanical systems[19];
  - Human motion prediction[20]

[16] Mauro Da Lio, Daniele Bortoluzzi, and Gastone Pietro Rosati Papini. "Modelling longitudinal vehicle dynamics with neural networks". In: *Vehicle System Dynamics* (2020).

[17] Mattia Piccinini et al. "A Physics-Driven Artificial Agent for Online Time-Optimal Vehicle Motion Planning and Control". In: *IEEE Access* (2023).

[18] Mauro Da Lio, Mattia Piccinini, and Francesco Biral. "Robust and Sample-Efficient Estimation of Vehicle Lateral Velocity Using Neural Networks With Explainable Structure Informed by Kinematic Principles". In: *IEEE Transactions on Intelligent Transportation Systems* (2023).

[19] Antonio Di Dino, Francesco Biral, and Paolo Bosetti. "Hybrid Modeling of Non-Linear Mechanical Systems: The Case of a Vehicle Shock Absorber". In: 2011.

[20] Alessandro Antonucci et al. "Efficient Prediction of Human Motion for Real-Time Robotics Applications With Physics-Inspired Neural Networks". In: *IEEE Access* (2022).

NNodely Framework

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- *Modeling*, *control* and *estimation* of **physical systems**, whose internal dynamics may be partially unknown

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- **Support professionals** with classical modeling backgrounds, such as **physicists** and **engineers**, in using data-driven approaches (but embedding knowledge inside) to address their challenges.

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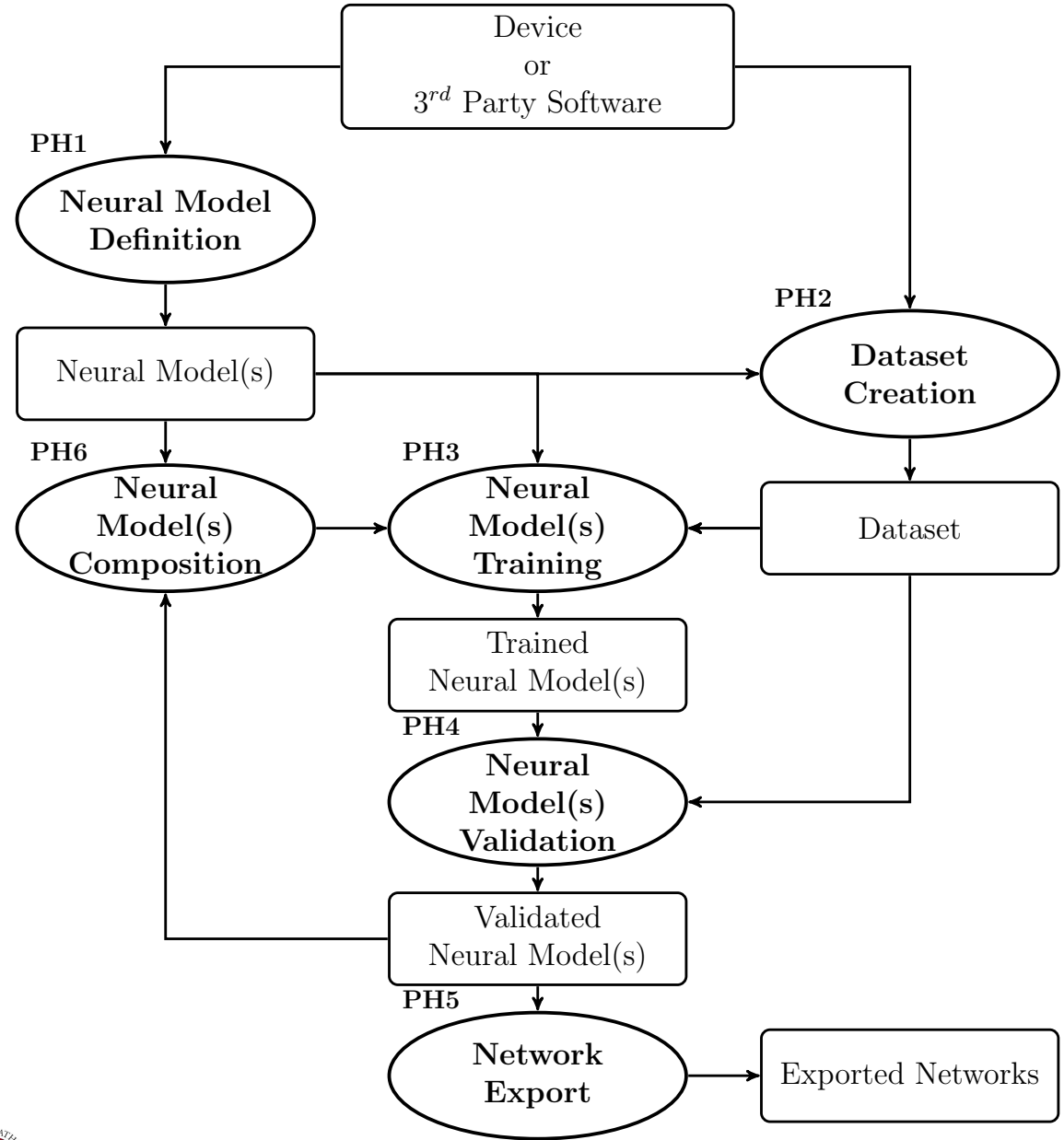
- A **repository** of incremental **know-how** that effectively collects approaches with the same purpose, i.e. building an increasingly advanced library of MS-NNs for various applications.

NNodely Framework

Workflow

Framework workflow



nnodely
neuralize your model

Model-Structured Neural Networks with nnodely

MS-NNs Definition (PH1)

- Defining **Inputs**
- Defining **Outputs**
- Defining **Relations**:
  - Aritmetic operations
  - Trigonometric operations
  - Custom functions
  - Local models
  - Fuzzification
  - ...

MS-NN Manipulation

- Data loading and dataset creation (PH2)
- Definition of the fitting objectives (PH3)
- Definition of the network composition and connection (PH6)
- Training (PH3)
- Validation using model based criteria (PH4)
- MS-NN export (PH5) in PyTorch and ONNX format

NNodely Framework

Physical Principles

The Principle

The **MS-NN** embeds and generalizes **physical principles** and prior-model knowledge, where the parameters are learned from **experimental data**

Embedding Physical Principles (Main Ideas)

Main nnodely concepts:

- Linear **superposition of forces**:

$$\dot{x} = f(x,u) = f_x(x) + f_1(x,u_1) + f_2(x,u_2) + \ldots + f_n(x,u_n)$$

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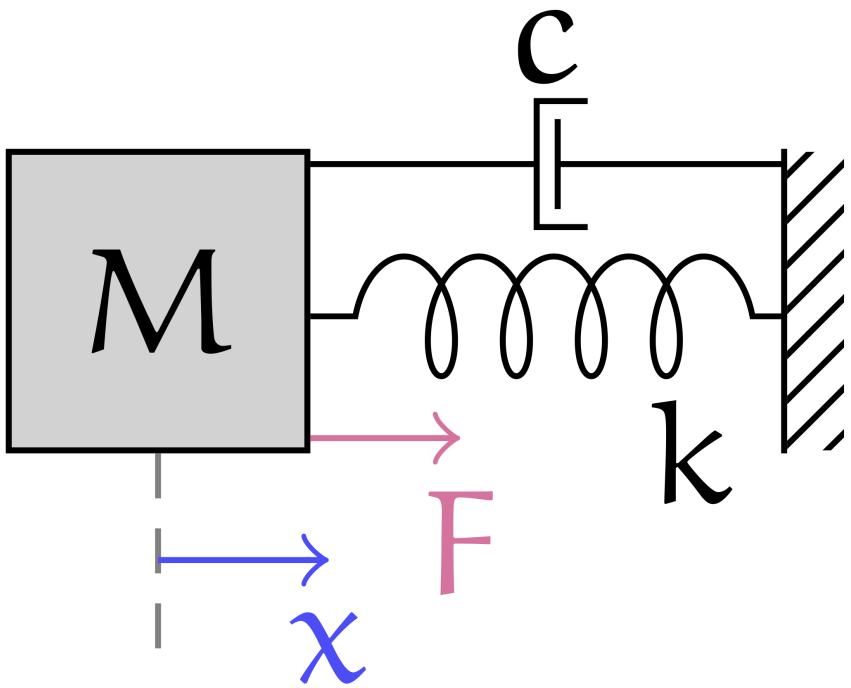
- Embedding easily the concept of **time** inside the NN
- Flexible managing of **recursive networks**

Use Cases

Simple example of a Mass-spring-damper

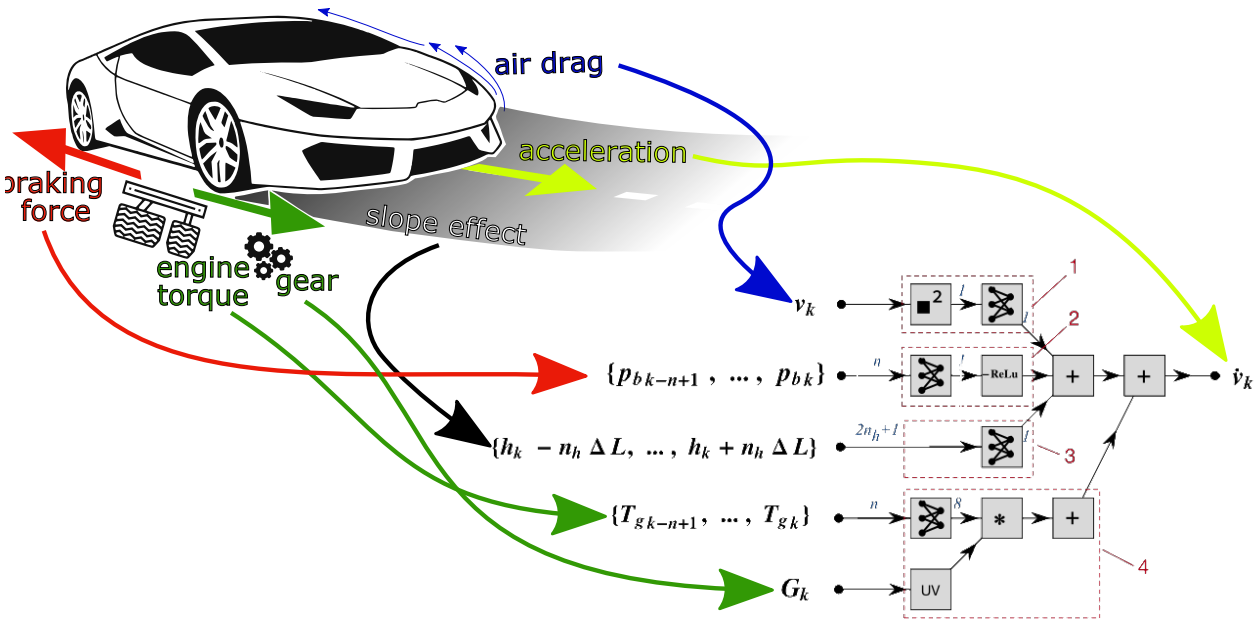
- Learn the dynamics of a mass-spring-damper system



$$x_{k+1} = \underbrace{\sum_{k=0}^{N_x-1} x[-k]\cdot h_x[(N_x-1)-k]}_{\mathrm{FIR}(\bar{x})} + \underbrace{F[0]\cdot h_F}_{\mathrm{FIR}(F)}$$

Modeling the forward longitudinal vehicle dynamics[21]

$$m\,\dot{v}_x = F_{x_f} + F_{x_r} - k_d v_x^2 - m\big(g c_r \cos(\theta) + g \sin(\theta)\big)$$

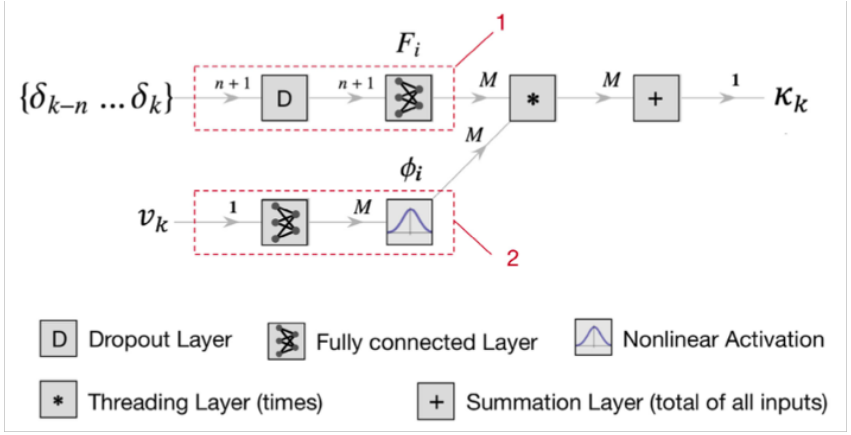


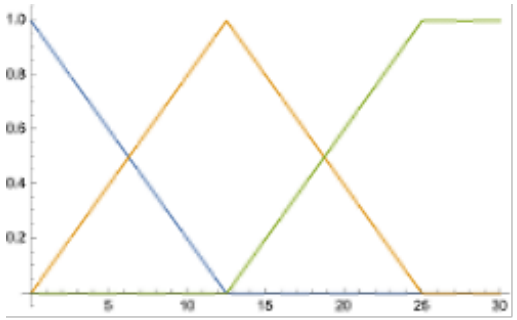
$$\dot{v}_x = \sum_i^{\text{gear}} \overbrace{g_i \text{FIR}_i(\bar{T}_g) - \text{Relu}(\text{FIR}(\bar{p_b}))}^{(F_{x_f}+F_{x_r})/m} + \overbrace{\text{FIR}(v_x^2)}^{k_d v_x^2/m} - \overbrace{\text{Linear}(\bar{h_k})}^{g c_r \cos(\theta)+g \sin(\theta)}$$

[21] Mauro Da Lio, Daniele Bortoluzzi, and Gastone Pietro Rosati Papini. "Modelling longitudinal vehicle dynamics with neural networks". In: *Vehicle System Dynamics* (2020).

Modeling the lateral vehicle dynamics

Forward model of a vehicle's lateral dynamics[22]



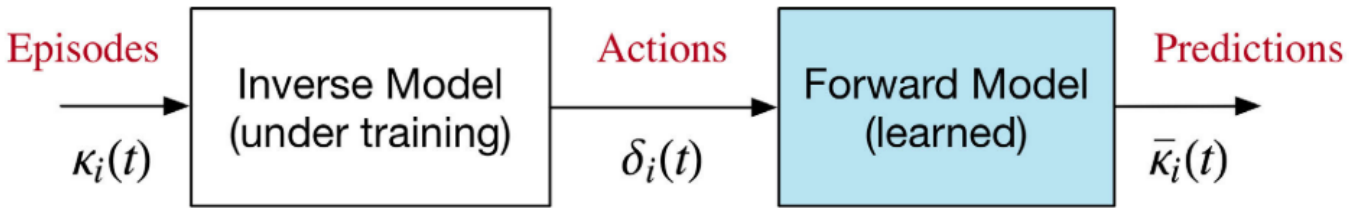


with $\phi_i(v) = \frac{1}{1+Av^2}\Lambda\left(\frac{v-v_i}{\Delta v}\right)$ where v_i are the centres of the receptive fields, Δv the receptive fields radius and $\Lambda(\cdot)$ is the Heaviside Lambda function: $\Lambda(x) = \max(1 - |x|, 0)$. The scaling factor $1 + Av^2$, with learnable A (understeering gradient)

[22] Mauro Da Lio et al. "A mental simulation approach for learning neural-network predictive control (in self-driving cars)". In: *IEEE Access* (2020).

Controlling the lateral vehicle dynamics

1. Train the **forward model** of the vehicle's lateral dynamics
2. Use the trained forward model to train the **inverse model**, which is a control system ⟶ unsupervised learning



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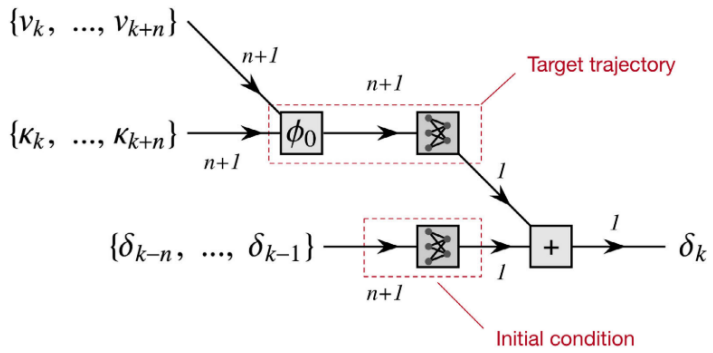
Inverse model of a vehicle's lateral dynamics[23]



with ϕ_0 threading v, and κ into $(1 + Av^2)\kappa$, which models the understeering gradient effect re-using the understeering coeffcient A from the forward dynamics

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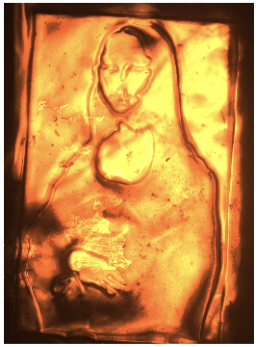
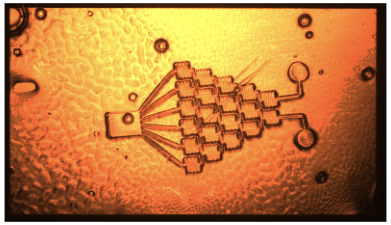
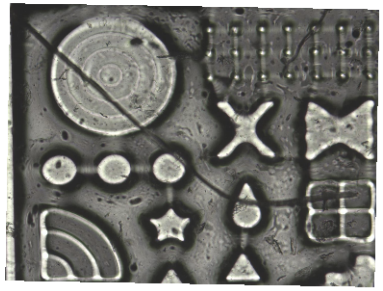
Controlling the 3D printing process

The network for defining the 3D printing process parameters.

$$\phi(t) = 1 - \exp^{-t^3 k}$$

Models nucleation and growth in crosslinking during polymerization.

$$d_c = D_p \log\left(\frac{E}{E_C}\right)$$

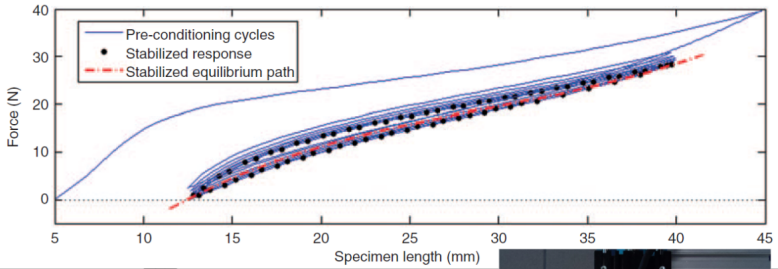
Describes how deep the resin will cure, depending on $\frac{E}{E_C}$.

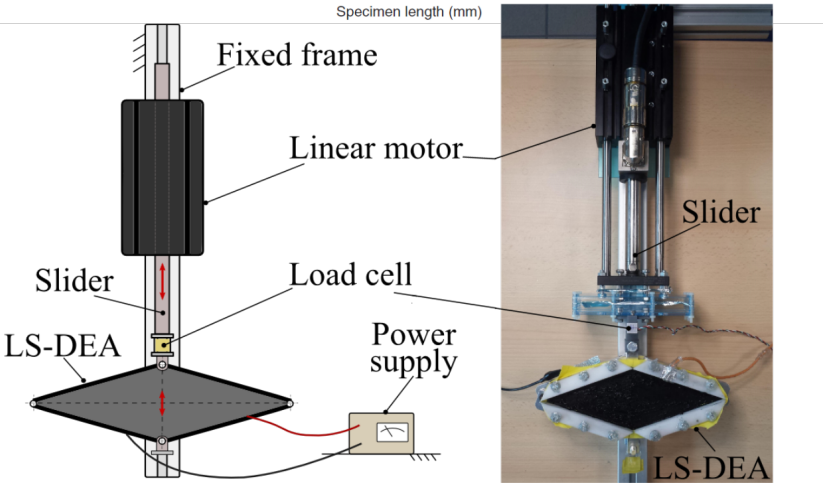
- Degree of polymerization $\phi(t)$ (unitless)
- Reaction rate constant k (s^{-n})
- Cure depth d_c (μm)
- Penetration depth D_p (μm)
- Delivered energy dose E (mJ/cm^2)
- Critical energy E_C (mJ/cm^2)

Model a response of electroactive polymers

The neural network model is base on a physical model of a viscoelastic material

$$f_{\text{tot}} = f_{\text{e}}(\lambda) + f_{\text{d}}\left([\lambda_t, \ldots, \lambda], [\dot{\lambda}_t, \ldots, \dot{\lambda}]\right) + f_{\text{v}}(V, \lambda)$$

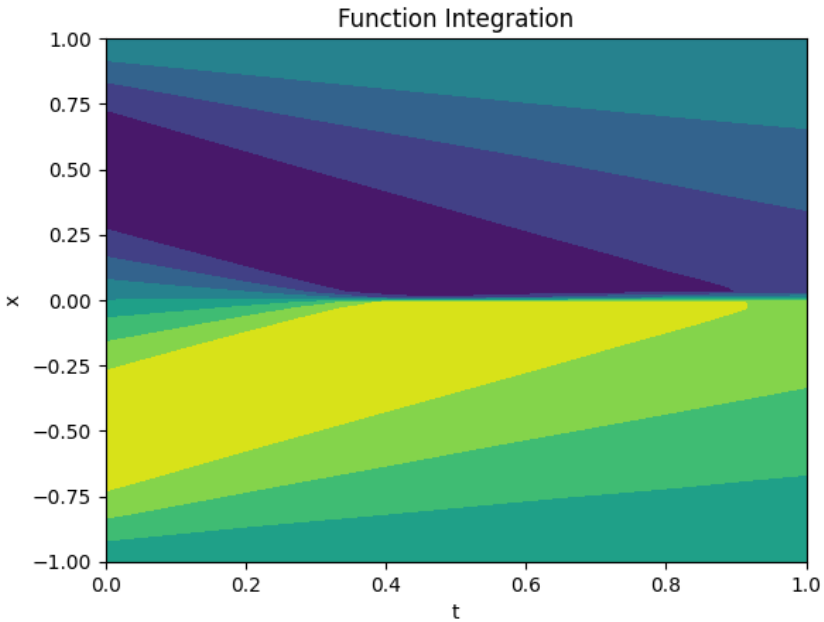




- total force realized: f_{tot}
- stretch: λ
- voltage: V
- elastic force: f_{e}
- viscoelastic and hysteretic force: f_{d}
- electric force: f_{v}

Integrate a nonlinear differential equation

Integrate the Burger's equation[24] in the range $x \in [-1, 1]$, $t \in [0, 1]$.



$$u = NN(t, x),$$

$$\frac{u}{dt} + u\frac{u}{dx} - \left(\frac{0.01}{\pi}\right)\frac{u}{dx^2} = 0,$$

$$u(0, x) = -\sin(\pi x),$$

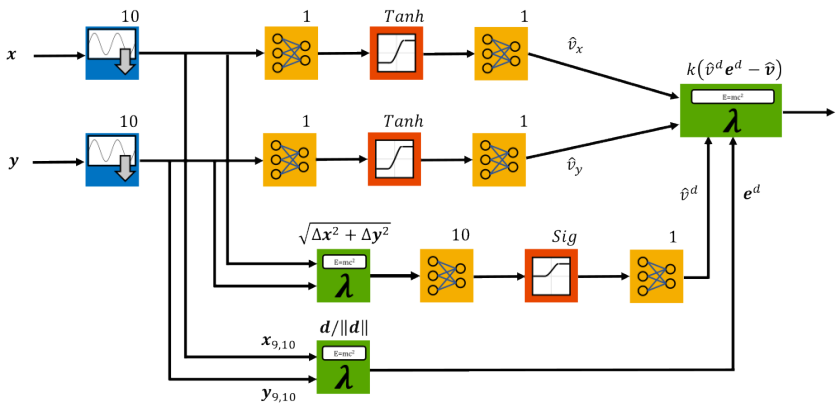
$$u(t, -1) = u(t, 1) = 0.$$

[24] M. Raissi, P. Perdikaris, and G.E. Karniadakis. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations". In: *Journal of Computational Physics* (2019).

Learning a pedestrian model

The network is based on social force model[25]

$$\mathbf{f}(t) = m\frac{v^d(t)\mathbf{e}^d(t) - \mathbf{v}(t)}{\tau} + \sum_w \mathbf{f}_w^W(t)$$



- forces on pedestrian: $\mathbf{f}$
- pedestrian mass: m
- pedestrian speed: $\mathbf{v}$
- desired velocity: v^d
- waypoint direction: $\mathbf{e}^d$
- velocity change rate: τ
- obstacle forces: $\mathbf{f}_w^W$

[25] Alessandro Antonucci et al. "Efficient Prediction of Human Motion for Real-Time Robotics Applications With Physics-Inspired Neural Networks". In: *IEEE Access* (2022).

NNodely-applications on github

The applications are available at

https://github.com/tonegas/nnodely-applications

Future Work

Future Work

- **Bridge the gaps** between machine learning and control theory.
- Apply nnodely to neuralize models and controllers from **different domains**;
- Starting from a nnodely model, **automatically** generate and train a nnodely **controller**.

modely

neuralize your model

Apply the framework on **your** task

and

 Star it if you like!

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