Breaking the curse of dimensionality in some control and parametric problems for PDEs

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Kick-off workshop of Working Group 2 "ML for CT"

Cost Action 24136
Interactions between Control Theory and Machine Learning

Working Group 2:
Machine Learning for Control Theory

Outline

1. **Machine Learning basis.** Where and why Machine-Learning-based methods may be useful in the numerical approximation of PDEs-based models?

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6. **Some related Open Problems**

Part I

Machine Learning Basis

Introduction: the set up of supervised learning

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2. Choose a loss function. If we are interested in fitting the data, a popular choice is the so-called **training error**

$$\hat{\mathcal{R}}_n(f) = \frac{1}{n}\sum_{i=1}^{n}\left(f(\boldsymbol{\theta}; \boldsymbol{x}_i) - f^*(\boldsymbol{x}_i)\right)^2, \quad f \in \mathcal{H}_m. \tag{1}$$

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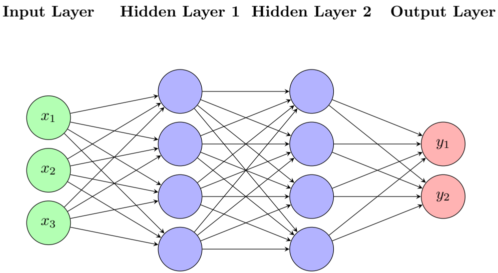
The overall objective is to minimize the **generalization error**

$$\mathcal{R}(f) = \mathbb{E}_{\boldsymbol{x}\sim\mathbb{P}}\left(f(\boldsymbol{\theta}; \boldsymbol{x}) - f^*(\boldsymbol{x})\right)^2, \quad f \in \mathcal{H}_m, \tag{2}$$

with $\mathbb{P}$ the (unknown) distribution of $\boldsymbol{x}$.

Hypothesis space: an example

A canonical example of an hypothesis space $\mathcal{H}_m$ (or a neural network architecture) is the so-called **Multi-Layer Perceptron (MLP)**.



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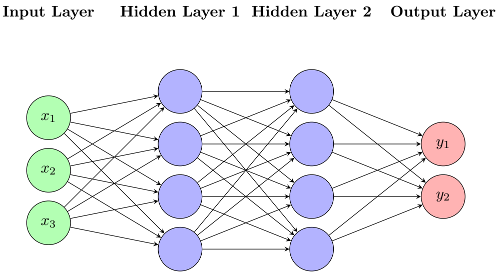

To each input $\boldsymbol{x} \in \mathbb{R}^d$ it associates the output $\boldsymbol{y} = f_m(\boldsymbol{x}) := \boldsymbol{x}^m$ defined by

$$\begin{cases} \text{input layer:} & \boldsymbol{x}^0 = \boldsymbol{x}, \\ \text{hidden layers:} & \boldsymbol{x}^{k+1} = \sigma\left(\omega^{k+1}\boldsymbol{x}^k + b^{k+1}\right) \quad \text{for } k = 0, 1, \cdots, m-2 \\ \text{output layer:} & \boldsymbol{x}^m = \omega^m \boldsymbol{x}^{m-1} + b^m, \end{cases}$$

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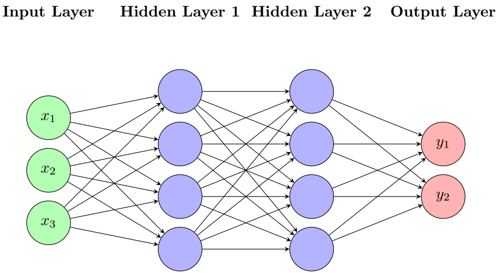

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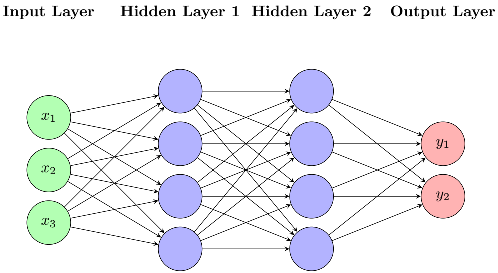

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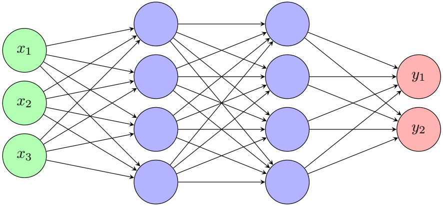

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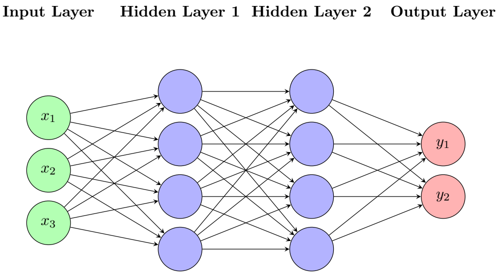

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Common choices include *rectifiers* such as ReLU: $\sigma(s) = \max\{s, 0\}$, and *sigmoids* such as $\sigma(s) = \tanh(s)$.

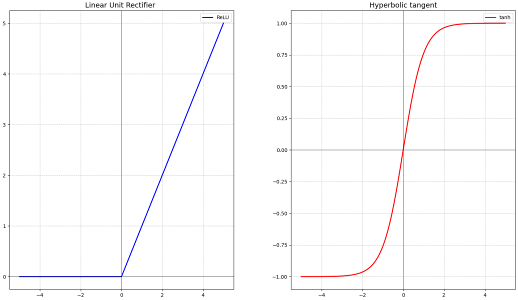

Figure: Linear Unit Rectifier (left) and hyperbolic tangent (right).

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- nonlinear Black- Scholes equation for pricing derivatives

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Machine learning is a promising tool to deal with high-dimensional problems

Part II

Physics Informed Neural Networks (PINNs)

A toy model: null control of the wave equation

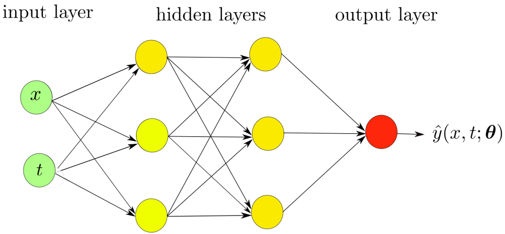
$$
\begin{cases}
y_{tt} - \Delta y = 0, & \text{in } Q_T \\
y(x,0) = y^0(x), & \text{in } \Omega \\
y_t(x,0) = y^1(x) & \text{in } \Omega \\
y(x,t) = 0, & \text{on } \Gamma_D \times (0,T) \\
y(x,t) = u(x,t) & \text{on } \Gamma_C \times (0,T)
\end{cases}
$$

Goal: Compute $u(x,t)$ such that

$$y(x,T) = y_t(x,T) = 0 \quad x \in \Omega.$$

Step 1: Neural network

A surrogate $\hat{y}(x, t; \boldsymbol{\theta})$ of the state variable $y(x, t)$ is constructed as



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\begin{cases}
\text{input layer:} & \boldsymbol{x}^0(\boldsymbol{x}) = \boldsymbol{x} = (x, t) \in \mathbb{R}^{d+1} \\
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\text{output layer:} & \boldsymbol{x}^m = \omega^m \boldsymbol{x}^{m-1} + b^m,
\end{cases}
$$

- $\omega^\ell \in \mathbb{R}^{N_\ell \times N_{\ell-1}}$ and $b^\ell \in \mathbb{R}^{N_\ell}$ are, respectively, the weights and biases so that $\boldsymbol{\theta} = \left\{\omega^\ell, b^\ell\right\}_{1 \leq \ell \leq m}$ are the parameters of the neural network, and
- σ is an activation function, e.g. $\sigma(s) = \tanh(s)$

Step 2: Training dataset

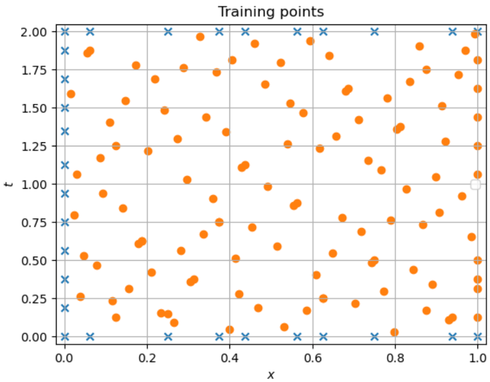

Figure: Illustration of a training dataset (based on Sobol points) in the domain $Q_2 = (0,1) \times (0,2)$. Interior points are marked with circles and boundary points in blue color. $\mathbf{x}_j = (x_j, t_j)$ are the features.

Step 3: **Loss function.** **Labels equal zero**

$$
\begin{aligned}
\mathcal{L}_{\text{int}}\left(\boldsymbol{\theta};\mathcal{T}_{\text{int}}\right) &= \sum_{j=1}^{N_{\text{int}}} w_{j,\text{int}}\left|\hat{y}_{tt}(\boldsymbol{x}_j;\boldsymbol{\theta}) - \Delta\hat{y}(\boldsymbol{x}_j;\boldsymbol{\theta})\right|^2, && \boldsymbol{x}_j \in \mathcal{T}_{\text{int}} \\
\mathcal{L}_{\Gamma_D}\left(\boldsymbol{\theta};\mathcal{T}_{\Gamma_D}\right) &= \sum_{j=1}^{N_b} w_{j,b}\left|\hat{y}(\boldsymbol{x}_j;\boldsymbol{\theta})\right|^2, && \boldsymbol{x}_j \in \mathcal{T}_{\Gamma_D} \\
\mathcal{L}^{\text{pos}}_{t=0}\left(\boldsymbol{\theta};\mathcal{T}_{t=0}\right) &= \sum_{j=1}^{N_0} w_{j,0}\left|\hat{y}(\boldsymbol{x}_j;\boldsymbol{\theta}) - y^0(\boldsymbol{x}_j)\right|^2, && \boldsymbol{x}_j \in \mathcal{T}_{t=0} \\
\mathcal{L}^{\text{vel}}_{t=0}\left(\boldsymbol{\theta};\mathcal{T}_{t=0}\right) &= \sum_{j=1}^{N_0} w_{j,0}\left|\hat{y}_t(\boldsymbol{x}_j;\boldsymbol{\theta}) - y^1(\boldsymbol{x}_j)\right|^2, && \boldsymbol{x}_j \in \mathcal{T}_{t=0} \\
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where $w_{j,\text{int}}$, $w_{j,b}$, $w_{j,0}$ and $w_{j,T}$ are the weights of suitable quadrature rules.

$$
\begin{aligned}
\mathcal{L}\left(\boldsymbol{\theta};\mathcal{T}\right) &= \lambda_1\mathcal{L}_{\text{int}}\left(\boldsymbol{\theta};\mathcal{T}_{\text{int}}\right) \\
&+\lambda_2\mathcal{L}_{\Gamma_D}\left(\boldsymbol{\theta};\mathcal{T}_{\Gamma_D}\right) \\
&+\lambda_3\mathcal{L}^{\text{pos}}_{t=0}\left(\boldsymbol{\theta};\mathcal{T}_{t=0}\right) + \lambda_4\mathcal{L}^{\text{vel}}_{t=0}\left(\boldsymbol{\theta};\mathcal{T}_{t=0}\right) \\
&+\lambda_5\mathcal{L}^{\text{pos}}_{t=T}\left(\boldsymbol{\theta};\mathcal{T}_{t=T}\right) + \lambda_6\mathcal{L}^{\text{vel}}_{t=T}\left(\boldsymbol{\theta};\mathcal{T}_{t=T}\right).
\end{aligned}
$$

Step 4: **Training process**

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{L}\left(\boldsymbol{\theta}; \mathcal{T}\right).$$

The approximation $\hat{u}(t; \boldsymbol{\theta}^*)$ of the control $u(x,t)$ is

$$\hat{u}(x,t;\boldsymbol{\theta}^*) = \hat{y}(x,t;\boldsymbol{\theta}^*), \quad x \in \Gamma_C,\ 0 \leq t \leq T.$$

Numerical approximation using PINNs

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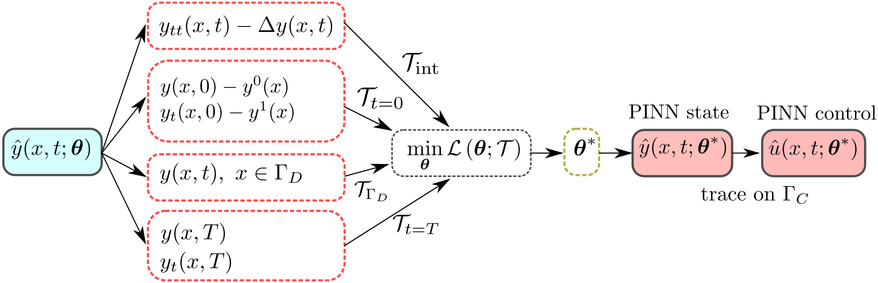
To sump up:



Why MLP is a suitable prediction model ?

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Let us consider the hypothesis space of single-layer neural nets

$$\mathcal{H}_m := \left\{ y_m(\boldsymbol{x}) := \sum_{i=1}^{m} a_i \sigma\left(\boldsymbol{\omega}_i \boldsymbol{x} + b_i\right) : \boldsymbol{x}, \boldsymbol{\omega}_i \in \mathbb{R}^{d+1}, a_i, b_i \in \mathbb{R} \right\}.$$

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Theorem (Pinkus Universal Approximation Theorem)

Let $f \in C^k(\mathbb{R}^{d+1})$. Assume that the activation function $\sigma \in C^k(\mathbb{R})$ is not a polynomial. Then, for any compact set $K \subset \mathbb{R}^{d+1}$ and any $\varepsilon > 0$ there exists $m \in \mathbb{N}$ and $y_m \in \mathcal{H}_m$ such that

$$\max_{\boldsymbol{x} \in K} \left| D^{\ell} f(\boldsymbol{x}) - D^{\ell} y_m(\boldsymbol{x}) \right| \leq \varepsilon$$

for all multiindex $\ell \leq k$. Moreover, each $a_i = a_i(f)$ is a continuous linear functional defined on K.

Pinkus, A.: *Approximation theory of the MLP model in neural networks* **Acta numer. 8**, 143-195, 1999.

Estimates on generalization error for the null control of the wave equation

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Training error

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\begin{aligned}
\mathcal{E}_{\text{train}} \quad &:= \mathcal{E}_{\text{train, int}} + \mathcal{E}_{\text{train, boundary}} + \mathcal{E}_{\text{train, initialpos}} + \mathcal{E}_{\text{train, initialvel}} \\
&+ \mathcal{E}_{\text{train, finalpos}} + \mathcal{E}_{\text{train, finalvel}},
\end{aligned}
$$

$$
\begin{cases}
\mathcal{E}_{\text{train, int}} & = \left(\mathcal{L}_{\text{int}}\left(\boldsymbol{\theta}^*; \mathcal{T}_{\text{int}}\right)\right)^{1/2} \\
\mathcal{E}_{\text{train, boundary}} & = \left(\mathcal{L}_{\Gamma_D}\left(\boldsymbol{\theta}^*; \mathcal{T}_{\Gamma_D}\right)\right)^{1/2} \\
\mathcal{E}_{\text{train, initialpos}} & = \left(\mathcal{L}^{\text{pos}}_{t=0}\left(\boldsymbol{\theta}^*; \mathcal{T}_{t=0}\right)\right)^{1/2} \\
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\mathcal{E}_{\text{train, finalpos}} & = \left(\mathcal{L}^{\text{pos}}_{t=T}\left(\boldsymbol{\theta}^*; \mathcal{T}_{t=T}\right)\right)^{1/2} \\
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\end{cases}
$$

Generalization error for control and state

$$
\begin{cases}
\mathcal{E}_{\text{gener}}(u) := \|u - \hat{u}\|_{L^2(\Gamma_C;(0,T))} \\
\mathcal{E}_{\text{gener}}(y) := \|y - \hat{y}\|_{C\left(0,T;L^2(\Omega)\right)\cap C^1\left(0,T;H^{-1}(\Omega)\right)}
\end{cases}
$$

Theorem (Estimates on generalization error)

Assume that both $y, \hat{y} \in C^2\left(\overline{Q_T}\right)$. *Then*

$$\begin{aligned}
\mathcal{E}_{gener}(u) \quad & \leq C \Big(\mathcal{E}_{train,\ int} + C_{q_{int}}^{1/2} N_{int}^{-\alpha_{int}/2} \\
& + \mathcal{E}_{train,\ boundary} + C_{qb}^{1/2} N_{b}^{-\alpha_{b}/2} \\
& + \mathcal{E}_{train,\ initialpos} + C_{qip}^{1/2} N_{0}^{-\alpha_{ip}/2} \\
& + \mathcal{E}_{train,\ initialvel} + C_{qiv}^{1/2} N_{0}^{-\alpha_{iv}/2} \\
& + \mathcal{E}_{train,\ finalpos} + C_{qfp}^{1/2} N_{T}^{-\alpha_{fp}/2} \\
& + \mathcal{E}_{train,\ finalvel} + C_{fv}^{1/2} N_{T}^{-\alpha_{fv}/2} \Big),
\end{aligned}$$

where $C = C(\Omega, T)$, *and consequently* $C = C(d)$ *also depends on the spatial dimension* d. *A similar estimate holds for the state variable.*
Moreover, training errors converge to zero as the size of the NN and the number of training points go to infinity.

García-Cervera, C., Kessler, M., Periago, F.: *Control of Partial Differential Equations via Physics-Informed Neural Networks* **J. Optim. Th. Appl. 196**, 391–414, 2023.

Part III

Numerical Implementation via DeepXDE

A few words on DeepXDE

Lu, Lu and Meng, Xuhui and Mao, Zhiping and Karniadakis, George Em: *DeepXDE: A deep learning library for solving differential equations* **SIAM Review 63**(1), 208–228, 2021.

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  https://github.com/lululxvi/deepxde
- For an introductory course focused on control of PDEs you may visit
  https://github.com/fperiago/pinn_deeponet_for_beginners

Experiment 1: control of the wave equation

Compute $u(t)$ such that the solution $y(x,t)$ of the problem

$$\begin{cases} y_{tt} - y_{xx} = 0, & \text{in } (0,1)\times(0,2) \\ y(x,0) = \sin(\pi x), & \text{in } (0,1) \\ y_t(x,0) = 0 & \text{in } (0,1) \\ y(0,t) = 0, & \text{on } (0,2) \\ y(1,t) = u(t) & \text{on } (0,2) \end{cases}$$

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This problem has an exact solution which can be obtained by means of D'Alembert formula. Indeed, by considering the function

$$\tilde{y^0}(x) = \begin{cases} \sin(\pi x) & -1 \leq x \leq 1 \\ 0 & \text{elsewhere,} \end{cases}$$

the explicit exact state is given by

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and the exact control is

$$u(t) = \begin{cases} \frac{1}{2} y^0(1-t) & 0 \le t \le 1 \\ -\frac{1}{2} y^0(t-1) & 1 \le t \le 2. \end{cases}$$

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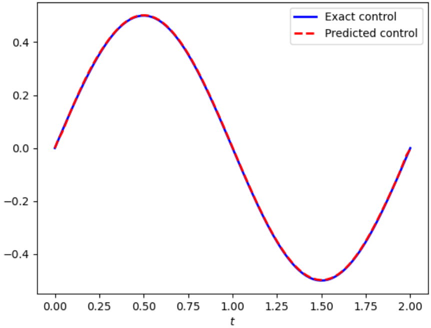

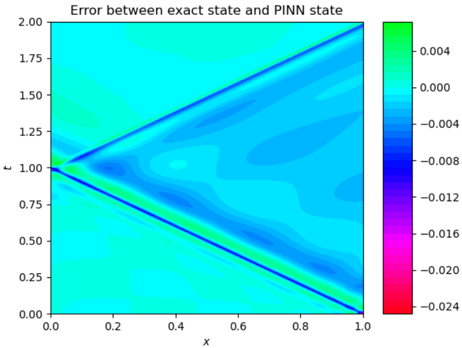

Figure: Experiment 1 (linear wave equation). Comparison between exact control $u(t)$ and PINN (or predicted) control $\hat{u}(t;\boldsymbol{\theta}^*)$ **(left)**, and error between exact state and PINN state, i.e. $y(x,t) - \hat{y}(x,t;\boldsymbol{\theta}^*)$ **(right)**. Neural network composed of 4 hidden layers and 50 neurons in each layer. No regularization. Number of training points $N = 10300$.

Part IV

Deep Operator Network (DeepONet)

Learning the controllability map

For the sake of clarity, we focus on the control problem

$$\begin{cases} y_{tt} - y_{xx} = 0, & \text{in } (0,1) \times (0,2) \\ y(x,0) = y^0(x), & \text{on } (0,1) \\ y_t(x,0) = y^1(x) & \text{on } (0,1) \\ y(0,t) = 0, & \text{on } (0,2) \\ y(1,t) = u(t) & \text{on } (0,2) \\ y(x,2) = y_t(x,2) = 0, & \text{on } (0,1). \end{cases}$$

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Goal: to approximate the controllabilty mapping

$$\begin{aligned} \mathcal{G}: \quad L^2(0,1)\times H^{-1}(0,1) &\to L^2(0,2) \\ (y^0, y^1) &\mapsto \mathcal{G}(y^0,y^1) := u \end{aligned}$$

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where u is the **unique** control of minimal L^2-norm.
The operator $\mathcal{G}$ is well-defined (uniqueness of the control), linear and continuous. Continuity is a consequence of the observability inequality

$$\|u\|_{L^2(0,2)} \le C\left(\|y^0\|_{L^2(0,1)} + \|y^1\|_{H^{-1}(0,1)}\right)$$

Thus, $\mathcal{G}$ is Lipschitz continuous.

- **Dataset**

  We fix a set of **sensor points** $\{x_1, x_2, \cdots, x_m\} \subset [0,1]$. The information of each selected continuous initial datum (y^0, y^1) is encoded in the vector

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- **Hypothesis space: the neural network**
  We will use the so-called **DeepONet**, which takes the form
  $$\mathcal{N}(\boldsymbol{\theta}; (y^{\text{initial}}(x_j); t)) := \sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k y^{\text{initial}}(x_j) + \theta_i^k \right) \cdot \sigma(w_k \cdot t + \eta_k)$$
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- **Loss function: Mean Squared Error (MSE)**

$$\text{MSE}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{\ell=1}^{N} |\mathcal{N}(\boldsymbol{\theta}; (y_\ell^{\text{initial}}; t_\ell)) - u_\ell|^2$$

DeepONet's architecture

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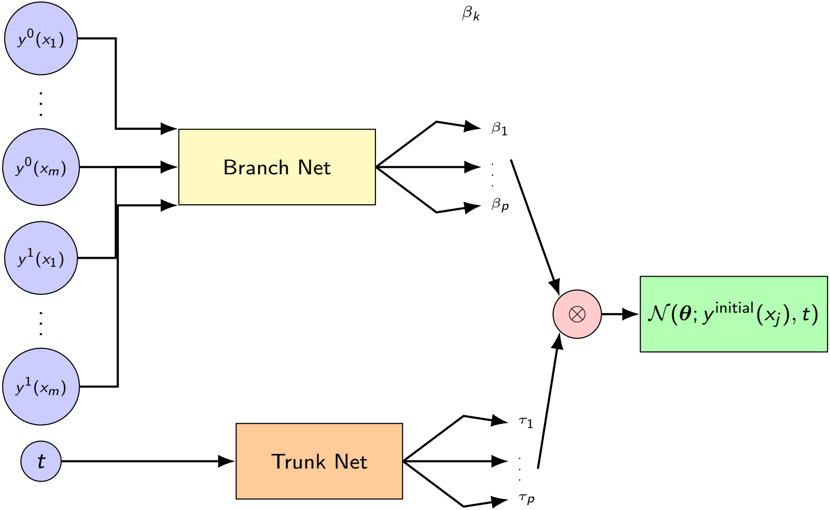

DeepONet's architecture

From a different perspective, the approximation scheme may be decomposed as

$$\begin{array}{ccc} X & \xrightarrow{\mathcal{G}} & Y \\ \downarrow \mathcal{E} & & \uparrow \mathcal{R} \\ \mathbb{R}^{2m} & \xrightarrow{\mathcal{A}} & \mathbb{R}^{p} \end{array}$$

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- $\mathcal{R} : \beta_k(y^{initial}) \mapsto \sum_{k=1}^{p} \beta_k(y^{\text{initial}})\tau_k(t)$ is a *reconstruction operator.*

Thus,

$$\mathcal{G} \approx \mathcal{R} \circ \mathcal{A} \circ \mathcal{E}.$$

DeepONet setup: Dataset

Definition (Data for DeepONet approximation)

Assume that $X \hookrightarrow L^2(D)$, and $Y \hookrightarrow L^2(U)$, for some Banach spaces X, Y. The pair $(\mu, \mathcal{G})$ is said to be **data for DeepONet approximation** provided $\mu \in \mathcal{P}_2(X)$ is Borel measurable with finite second moments, there exists a Borel set $A \subset X$, composed of continuous functions, $\mu(A) = 1$, and $\mathcal{G} : X \to Y$ is a Borel measurable mapping with $\|\mathcal{G}\|_{L^2(\mu)} < \infty$.

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How to sample continuous functions for the initial data (y^0, y^1) ?

We choose $\mu \in \mathcal{P}\left(C(0,1)\right)$ a probability measure whose probability law is given by a Karhunen-Loève expansion

$$\mu \sim \sum_{j=1}^{\infty} \sqrt{\lambda_j} \xi_j(\omega) \varphi_j(x) \tag{3}$$

We take $\xi_j \sim \mathcal{N}(0,1)$ i.i.d. standard Gaussian variables, and (λ_j, φ_j) are the eigenvalues and normalized eigenfuncions of the operator

$$\mathcal{C}(\phi)(x) = \int_0^1 C(x, x')\phi(x')\, dx', \quad C(x, x') = \sigma^2 \exp\left(-\frac{|x - x'|^2}{2\ell^2}\right)$$

DeepONet setup: Dataset

Definition (Data for DeepONet approximation)

Assume that $X \hookrightarrow L^2(D)$, and $Y \hookrightarrow L^2(U)$, for some Banach spaces X, Y. The pair $(\mu, \mathcal{G})$ is said to be **data for DeepONet approximation** provided $\mu \in \mathcal{P}_2(X)$ is Borel measurable with finite second moments, there exists a Borel set $A \subset X$, composed of continuous functions, $\mu(A) = 1$, and $\mathcal{G} : X \to Y$ is a Borel measurable mapping with $\|\mathcal{G}\|_{L^2(\mu)} < \infty$.

We need an **encoding operator** $\mathcal{E} : X \to \mathbb{R}^m$ to represent functions as vectors

How to sample continuous functions for the initial data (y^0, y^1) ?

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Thus, we truncate (3) and sample the Gaussian random variables. Remember that by Mercer's theorem $\{\varphi_j\}$ is an ortonormal basis of $L^2(0,1)$.

DeepONet setup: Dataset

After fixing a set of **sensor points** $\{x_1, x_2, \cdots, x_m\} \subset [0,1]$, the information of each selected continuous initial datum (y^0, y^1) is **encoded** in the vector

$$(y^0(x_1), y^0(x_2), \cdots, y^0(x_m); y^1(x_1), y^1(x_2), \cdots, y^1(x_m)) \equiv y^{\text{initial}}$$

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Putting all together, the **training dataset** is

$$\{(y_{jk}^{\text{initial}}; u_j(t)), 1 \le j \le N, 1 \le k \le 2m\},$$

evaluated at a finite selection of times t. Precisely,

$$\left[\begin{array}{cccc}
y_{1,1}^{\text{initial}} & \cdots & y_{1,2m}^{\text{initial}} & u_1(t_1) \\
\cdots & \cdots & \cdots & \cdots \\
y_{1,1}^{\text{initial}} & \cdots & y_{1,2m}^{\text{initial}} & u_1(t_\ell) \\
\hline
\cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots \\
\hline
y_{N,1}^{\text{initial}} & \cdots & y_{N,2m}^{\text{initial}} & u_N(t_1) \\
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\end{array}\right]$$

Experiment 2: Smooth initial conditions

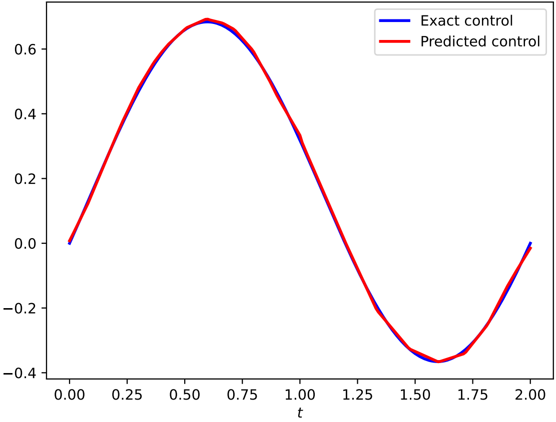

Figure: Experiment 2: wave equation. Exact versus predicted solutions for the smooth initial conditions $y^0(x) = y^1(x) = \sin(\pi x)$. $n_{functions} = 10^4$, $(\ell_0, \ell_1) = (0.25, 0.125)$, $n_{sensors} = 101$, $p = 40$. Relative error $\approx 1\%$.

Experiment 3: Unsmooth initial conditions

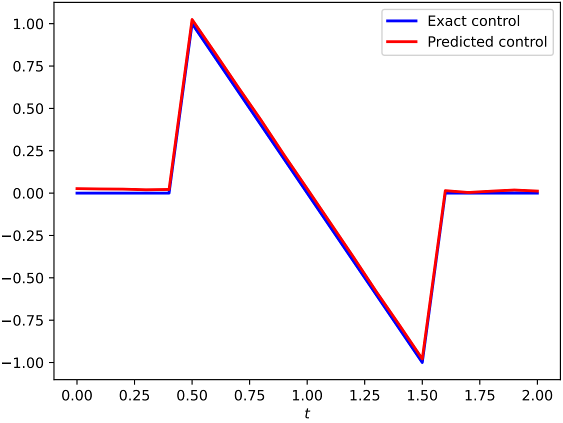

Figure: Experiment 3: wave equation. Exact versus predicted solutions for the unsmooth initial conditions $y^0(x) = \begin{cases} 4x, & 0 \leq x \leq 0.5 \\ 0, & 0.5 < x \leq 1 \end{cases}, \quad y^1(x) = 0.$

$n_{functions} = 10^4$, $(\ell_0, \ell_1) = (0.03125, 0.03125)$, $p = 100$. $n_{sensors} = 11$. Relative error $\approx 4\%$.

Part V

The curse of Dimensionality (CoD)

Curse of dimensionality

Let $f \in H^\alpha$ and let f_m be a two-layer approximation of f.

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Approximation error (due to the choice of $\mathcal{H}_m$): typically

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If $m^{-\alpha/d} = 0.1$, then $m = 10^{d/\alpha} = 10^d$, if $\alpha = 1$. **Curse of Dimensionality**

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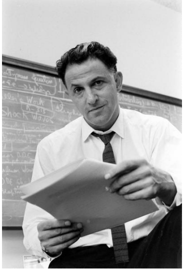

... a computational solution ... is quite definitely not routine when the number of variables is large. All this may be subsumed under the heading
Curse of Dimensionality.
R. Bellman. Dynamic Programming, 1957.

When we talk about error, what are we talking about?

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- **Approximation error:** This is the distance between the Hypothesis space and the operator $\mathcal{G}$ to be approximated, i.e., if $\mathcal{F}$ is a fixed space of DeepONets, then

$$\mathcal{N}_{\mathcal{F}} = \arg\min_{\mathcal{N}\in\mathcal{F}} \mathcal{L}(\mathcal{N}) := \int_{L^2(D)}\int_U |\mathcal{G}(y)(t) - \mathcal{N}(y)(t)|^2 \, dt d\mu(y),$$

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- **Generalization (or estimation) error:** We approximate $\mathcal{N}_{\mathcal{F}}$ by using a specific (training) dataset $\mathcal{T}$, and a **empirical loss**. So, we get

$$\mathcal{N}_{\mathcal{T}} = \arg\min_{\mathcal{N}\in\mathcal{F}} \mathcal{L}_M(\mathcal{N}) := \frac{|U|}{M} \sum_{j=1}^{M} |\mathcal{G}(y_j)(t_j) - \mathcal{N}(y_j)(t_j)|^2$$

Thus, $\mathcal{E}_{\text{gener}} := (\mathcal{L}(\mathcal{N}_{\mathcal{T}}) - \mathcal{L}(\mathcal{N}_{\mathcal{F}}))^{1/2}$.

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- **Optimization error:** The empirical loss is highly nonlinear, non-convex so that we compute a local minimum $\mathcal{N}_M$ of $\mathcal{L}_M$. Optimization error is then

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Error analysis and the curse of dimensionality

$$\mathcal{E}_{\text{total}} = \mathcal{E}_{\text{approx}} + \mathcal{E}_{\text{gener}} + \mathcal{E}_{\text{optim}}$$

Definition (Curse of dimensionality)

For a given $\varepsilon > 0$, let $\mathcal{N}_\varepsilon$ be a DeepONet such that $\mathcal{E}_{\text{approx}} < \varepsilon$, and

$$\text{size}\left(\mathcal{N}_\varepsilon\right) \sim \mathcal{O}\left(\varepsilon^{-\vartheta_\varepsilon}\right) \quad \text{for some } \vartheta_\varepsilon \geq 0.$$

Our DeepONet approximation, with underlying measure μ, is said to *incurr a curse of dimensionality* if $\lim_{\varepsilon\to 0} \vartheta_\varepsilon = +\infty$ and *breaks the curse of dimensionality* if $\lim_{\varepsilon\to 0} \vartheta_\varepsilon = \overline{\vartheta} < +\infty$.

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Yarotsky proved that the approximation of a general Lipschitz function to accuracy ε requires a ReLU network of size[1] $\varepsilon^{-m(\varepsilon)/2}$, with $m(\varepsilon) \to \infty$ as $\varepsilon \to 0$, and hence suffers from the curse of dimensionality.

Yarotsky, D.: *Optimal approximation of continuous functions by very deep relu networks.* **Conference on Learning Theory. PMLR,** 639-649, 2018.

In our setting, m is the number of sensors for the enconding operator $u \mapsto \mathcal{E}(u) = (u(x_1), \cdots, u(x_m))$.

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Error analysis and the curse of dimensionality

However, for some classes of linear and nonlinear operators, the DeepONet approximation may break the curse of dimensionality for **approximation error.**

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- bounded linear operators $\mathcal{G} : L^2(D) \to L^2(U)$

Application to our controllability setting

Set $\mathbb{T} = [0, \pi]$. Consider the operator

$$\mathcal{G} : L^2(\mathbb{T}) \times H^{-1}(\mathbb{T}) \to L^2(0, 4\pi), \quad (y^0, y^1) \mapsto \mathcal{G}(y^0, y^1) = u$$

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The key ingredient here is that in the decomposition

$$\begin{array}{ccc} X & \xrightarrow{\mathcal{G}} & Y \\ \downarrow \mathcal{E} & & \uparrow \mathcal{R} \\ \mathbb{R}^{2m} & \xrightarrow{\mathcal{A}} & \mathbb{R}^p \end{array}$$

the error associated with the linear operator $\mathcal{A}$ vanishes since if σ is an ReLU activation function, then

$$\mathcal{A}x + b = \sigma(\mathcal{A}x + b) - \sigma(-(\mathcal{A}x + b)).$$

Theorem (DeepONet approximation of controllability systems)

Consider the control system for $x \in \Omega \subset \mathbb{R}^d$ *and* $t > 0$*:*

$$\begin{cases} y' + Ay = 1_\omega u \\ y(0) = y^0 \end{cases}$$

and assume that for some $T > 0$ *there exists a unique control* $u \in L^2(\omega \times (0,T))$ *such that* $y(T) = 0$.
Consider the operator $\mathcal{G} : y^0 \to u$*. Then, for any fixed* $\varepsilon > 0$ *and* $\sigma > 0$*, there exists a DeepONet* $\mathcal{N} = (\beta, \tau)$ *achieving an approximation error*

$$\mathcal{E}_{approx} = \|\mathcal{G} - \mathcal{N}\|_{L^2(\mu)} \lesssim \varepsilon$$

and such that

$$size(\beta) \lesssim \log(\varepsilon^{-1}), \quad depth(\beta) \lesssim 1, \quad p \sim \log(\varepsilon^{-1})^d, \quad m \sim \log(\varepsilon^{-1})^{2d+\sigma}.$$

García-Cervera, C.J.; Kessler, M.; Pedregal, P.; Periago, F.: *Universal Approximation of Set-Valued Maps and Application to Control.* **Submitted,** 2025.

Estimates for generalization error for DeepONet

Boundedness assumption: there exists $\psi : L^2(D) \to [0, +\infty[$ such that

$$|\mathcal{G}(y)(t)| \leq \psi(y), \qquad \sup_{\theta \in [-B,B]^{d_\theta}} |\mathcal{N}_\theta(y)(t)| \leq \psi(y), \quad \forall y \in L^2(D), \forall t \in U,$$

and there exists $C, \kappa > 0$ such that

$$\psi(y) \leq C \left(1 + \|y\|_{L^2(D)}\right)^\kappa .$$

Lipschitz continuity assumption: there exists $\Phi : L^2(D) \to [0, +\infty[$ such that

$$|\mathcal{N}_\theta(y)(t) - \mathcal{N}_{\theta'}(y)(t)| \leq \Phi(y)\|\theta - \theta'\|_{\ell^\infty}, \quad \forall y \in L^2(D), \forall t \in U,$$

and there exists $C, \kappa > 0$ such that

$$\Phi(y) \leq C \left(1 + \|y\|_{L^2(D)}\right)^\kappa .$$

Theorem (Bound for generalization error)

Let $\mathcal{N}_\mathcal{F}$ and $\mathcal{N}_\mathcal{T}$ be as before. If the above two assumptions hold, then

$$\mathbb{E}\left[\mathcal{L}(\mathcal{N}_\mathcal{T}) - \mathcal{L}(\mathcal{N}_\mathcal{F})\right] \leq \frac{C}{\sqrt{N}} \left(1 + C d_\theta \log\left(CB\sqrt{N}\right)\right)^{2\kappa + \frac{1}{2}} \tag{4}$$

where the constant $C = C(\mu, \psi, \Phi)$ is independent of B and d_θ.

Part VI

Open problems

Open problem 1

Consider a control system:

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Open problem 1: learn this map with ML tools

Hint: a class of set-valued neural networks called **SIMONet** has been introduced in

García-Cervera, C.J.; Kessler, M.; Pedregal, P.; Periago, F.: *Universal Approximation of Set-Valued Maps and Application to Control.* **Submitted,** 2025.

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Open problem 1: learn this map with ML tools

Hint: a class of set-valued neural networks called **SIMONet** has been introduced in

García-Cervera, C.J.; Kessler, M.; Pedregal, P.; Periago, F.: *Universal Approximation of Set-Valued Maps and Application to Control.* **Submitted,** 2025.

Required skills for applicants: Good command of Python and a basic knowledge of control theory

Open problem 1

Consider a control system:

$$\begin{cases} y' + Ay = Bu \\ y(0) = y^0 \end{cases}$$

The mapping

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Contact person: Francisco Periago. Email: f.periago@upct.es

Open problem 2

A two-layer neural network may be represented as

$$f_m(\boldsymbol{x}) = \frac{1}{m} \sum_{j=1}^{m} a_j \sigma \left(\boldsymbol{\omega}_j^T \boldsymbol{x} + b_j \right) \tag{5}$$

where $(a_j, \boldsymbol{\omega}_j, b_j)$ are the parameters and σ is the activation function.

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$$f_\rho(\boldsymbol{x}) = \int_{\mathbb{R}^{d+2}} a\sigma\left(\boldsymbol{\omega}^T \boldsymbol{x} + b\right)\, \rho\left(da, d\boldsymbol{\omega}, db\right) = \mathbb{E}_\rho\left[a\sigma(\boldsymbol{\omega}^T \boldsymbol{x})\right]$$

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Definition (Barron space)

Let $\sigma(x) = \max\{0, x\}$ be the ReLU activation function. Barron space $\mathcal{B}$ is the one composed of continuous functions that admit a representation in the form

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ρ being a probability distribution on $\left(\mathbb{R} \times \mathbb{R}^d \times \mathbb{R}, \Sigma\right)$, and, in addition, its norm

$$\|f\|_{\mathcal{B}} := \inf_{\rho} \max_{(a,\boldsymbol{w},b)\in \text{supp }(\rho)} |a|\left(\|\boldsymbol{\omega}\|_1 + |b|\right)$$

is finite.

Open problem 2

Theorem (Direct approximation)

For any $f \in \mathcal{B}$ and $m \in \mathbb{N}$, there exists a two-layer neural network $f_m(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{m}\sum_{j=1}^m a_j \sigma\left(\boldsymbol{\omega}_j^T \boldsymbol{x} + b_j\right)$, with m neurons $\boldsymbol{\theta} = (a_j, \boldsymbol{\omega}_j, b_j)$ such that

$$\|f - f_m\|_{L^2}^2 \leq 3\frac{\|f\|_{\mathcal{B}}^2}{m}.$$

Moreover,

$$\|\boldsymbol{\theta}\| := \frac{1}{m}\sum_{j=1}^m |a_j| \left(\|\boldsymbol{\omega}_j\|_1 + |b_j|\right) \leq 2\|f\|_{\mathcal{B}}.$$

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Application to high-dimensional PDEs

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Application to high-dimensional PDEs

Proposition

Let $\sigma(z) = \max\{z, 0\}$ and $g(x) = \sigma(x_1)$ be a Barron function on $\mathbb{R}^d$, $d \geq 2$. Denote by B^d the unit ball in $\mathbb{R}^d$ and by u the solution to

$$\begin{cases} -\Delta u = 0 & \text{in} \quad B^d \\ u = g & \text{on} \quad \partial B^d. \end{cases}$$

If $d \geq 3$, then u is not a Barron function on B^d.

Open problem 2

Open problem 2: regularity theory for PDEs in high dimensions

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Weinan E, Chao Ma, Lei Wu : *The Barron Space and the Flow-Induced Function Spaces for Neural Network Models* **Constructive Approximation,** Vol. 55, 369–406, 2022.

Weinan E. and S. Wojtowytsch: *Some observations on high-dimensional PDEs with Barron data.* **Proceedings of Machine Learning Research,** Vol. 107, 253–269, 2021.

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Thank you for your attention !