An introduction to deep-learning-based methods for optimization and control of PDEs

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XXI Jacques-Louis Lions Hispano-French School on Numerical Simulation in Physics and Engineering

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Outline of the course

- **Part I: 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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- **Part IV: Numerical implementation via DeepXDE.** A Python library for scientific machine learning and physics-informed learning

Part I

Machine Learning Basis

Introduction: the set up of supervised learning

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

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

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

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

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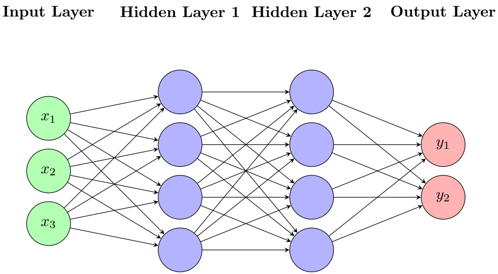
A canonical example of an hypothesis space $\mathcal{H}_m$ (or a neural network architecture) is the so-called **Multi-Layer Perceptron (MLP)**.



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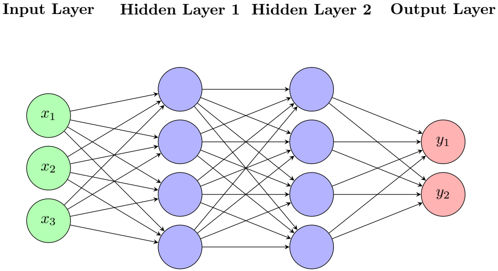

To each input $\boldsymbol{x} \in \mathbb{R}^d$ it associates the output $\boldsymbol{y} = f_m(\boldsymbol{x}) := \boldsymbol{x}^m$ defined by

$$\begin{cases} \boldsymbol{x}^{k+1} = \sigma\left(\omega^k \boldsymbol{x}^k + b^k\right) \quad \text{for } k = 0, 1, \cdots, m-1 \\ \boldsymbol{x}^0 = \boldsymbol{x}, \end{cases} \tag{3}$$

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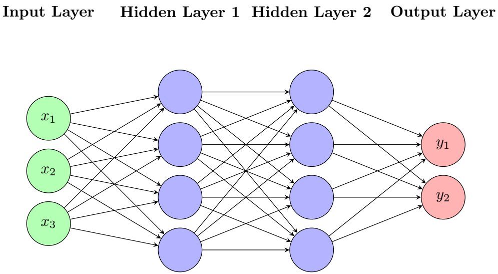

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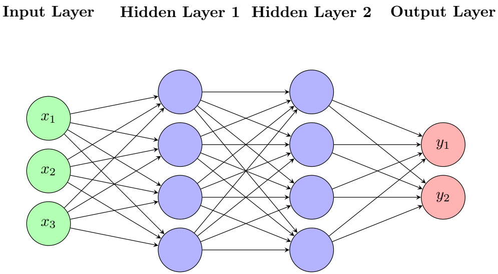

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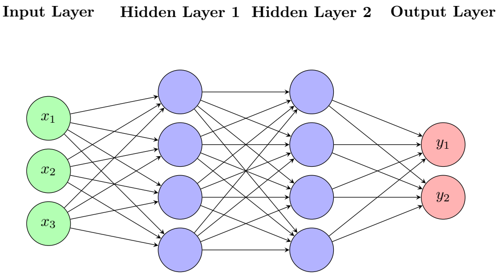

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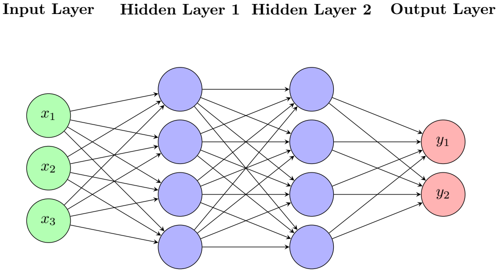

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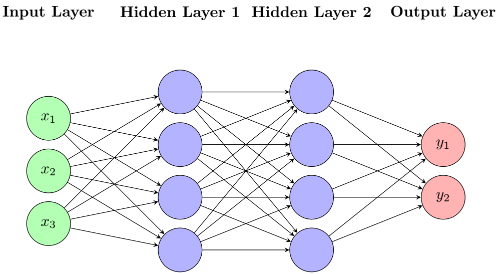

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Common choices include *rectifiers* such as ReLU: $\sigma(s) = \max\{s, 0\}$, and *sigmoids* such as $\sigma(s) = \tanh(s)$.

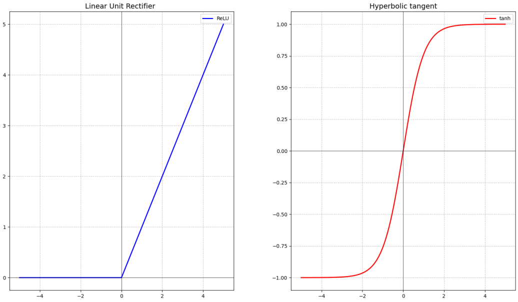

Figure: Linear Unit Rectifier (left) and hyperbolic tangent (right).

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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

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Part II

Physics Informed Neural Networks (PINNs)

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A toy model: null control of the wave equation

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

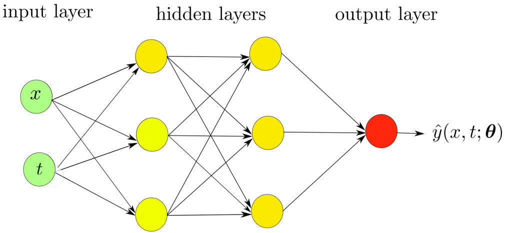
Goal: Compute $u(x,t)$ such that

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

Numerical approximation using PINNs

Step 1: Neural network

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



$$\begin{cases} \text{input layer:} & \mathcal{N}^0(\boldsymbol{x}) = \boldsymbol{x} = (x, t) \in \mathbb{R}^{d+1} \\ \text{hidden layers:} & \mathcal{N}^\ell(\boldsymbol{x}) = \sigma\left(\boldsymbol{W}^\ell \mathcal{N}^{\ell-1}(\boldsymbol{x}) + \boldsymbol{b}^\ell\right) \in \mathbb{R}^{N_\ell}, \quad \ell = 1, \cdots, L-1 \\ \text{output layer:} & \hat{y}\left(\boldsymbol{x}; \boldsymbol{\theta}\right) = \mathcal{N}^L(\boldsymbol{x}) = \boldsymbol{W}^L \mathcal{N}^{L-1}(\boldsymbol{x}) + \boldsymbol{b}^L \in \mathbb{R} \end{cases}$$

- $\mathcal{N}^\ell : \mathbb{R}^{d_{in}} \to \mathbb{R}^{d_{out}}$ is the ℓ layer with N_ℓ neurons,
- $\boldsymbol{W}^\ell \in \mathbb{R}^{N_\ell \times N_{\ell-1}}$ and $\boldsymbol{b}^\ell \in \mathbb{R}^{N_\ell}$ are, respectively, the weights and biases so that $\boldsymbol{\theta} = \left\{\boldsymbol{W}^\ell, \boldsymbol{b}^\ell\right\}_{1 \le \ell \le L}$ are the parameters of the neural network, and
- σ is an activation function, e.g. $\sigma(s) = \tanh(s)$

Numerical approximation using PINNs

Step 2: Training dataset

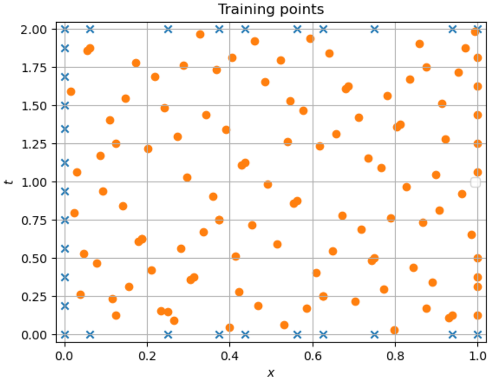


Figure: Illustration of a training dataset (based on Sobol points) in the domain $Q_2 = (0,1) \times (0,2)$. Interior points are marked with circles and boundary points in blue color. $\mathbf{x}_j = (x_j, t_j)$ are the features.

Numerical approximation using PINNs

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

$$
\begin{aligned}
\mathcal{L}_{\text{int}}\left(\boldsymbol{\theta}; \mathcal{T}_{\text{int}}\right) &= \textstyle\sum_{j=1}^{N_{\text{int}}} w_{j,\text{int}} |\hat{y}_{tt}(\boldsymbol{x}_j; \boldsymbol{\theta}) - \Delta \hat{y}(\boldsymbol{x}_j; \boldsymbol{\theta})|^2, && \boldsymbol{x}_j \in \mathcal{T}_{\text{int}} \\
\mathcal{L}_{\Gamma_D}\left(\boldsymbol{\theta}; \mathcal{T}_{\Gamma_D}\right) &= \textstyle\sum_{j=1}^{N_b} w_{j,b} |\hat{y}(\boldsymbol{x}_j; \boldsymbol{\theta})|^2, && \boldsymbol{x}_j \in \mathcal{T}_{\Gamma_D} \\
\mathcal{L}^{\text{pos}}_{t=0}\left(\boldsymbol{\theta}; \mathcal{T}_{t=0}\right) &= \textstyle\sum_{j=1}^{N_0} w_{j,0} |\hat{y}(\boldsymbol{x}_j; \boldsymbol{\theta}) - y^0(\boldsymbol{x}_j)|^2, && \boldsymbol{x}_j \in \mathcal{T}_{t=0} \\
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\mathcal{L}^{\text{pos}}_{t=T}\left(\boldsymbol{\theta}; \mathcal{T}_{t=T}\right) &= \textstyle\sum_{j=1}^{N_T} w_{j,T} |\hat{y}(\boldsymbol{x}_j; \boldsymbol{\theta})|^2, && \boldsymbol{x}_j \in \mathcal{T}_{t=T} \\
\mathcal{L}^{\text{vel}}_{t=T}\left(\boldsymbol{\theta}; \mathcal{T}_{t=T}\right) &= \textstyle\sum_{j=1}^{N_T} w_{j,T} |\hat{y}_t(\boldsymbol{x}_j; \boldsymbol{\theta})|^2, && \boldsymbol{x}_j \in \mathcal{T}_{t=T},
\end{aligned}
$$

where $w_{j,\text{int}}$, $w_{j,b}$, $w_{j,0}$ and $w_{j,T}$ are the weights of suitable quadrature rules.

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

Numerical approximation using PINNs

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

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

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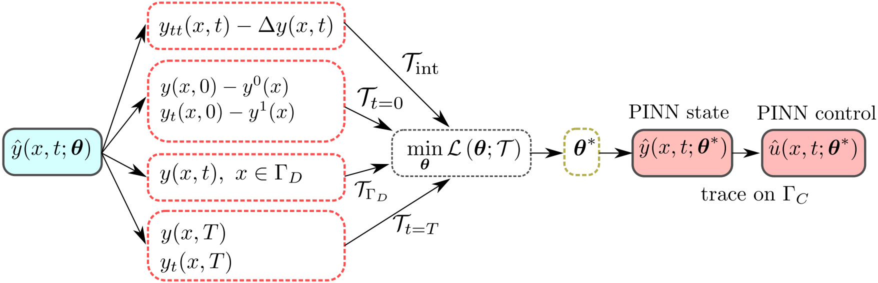
To sump up:



Approximation theory and convergence analysis

Why MLP is a suitable prediction model ?

Approximation theory and convergence analysis

Why MLP is a suitable prediction model ?

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.

Why is so crucial that the activation function not to be a polynomial?

Approximation theory and convergence analysis

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If σ is a polynomial of degree m, then $\sigma(\omega x + b)$ is a polynomial of total degree at most m. Thus, $\mathcal{H}_m$ is the space of all polynomials of degree m, which is not dense in $C(K)$, $K \subset \mathbb{R}$ compact.

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Conversely, let $\sigma\in C^{\infty}(\mathbb{R})$. Consider the space

$$\mathcal{N}\left(\sigma;\mathbb{R},\mathbb{R}\right)=\mathrm{span}\left\{\sigma(wx+b),\quad w,b\in\mathbb{R}\right\}.$$

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$$\mathcal{N}(\sigma; \mathbb{R}, \mathbb{R}) = \operatorname{span}\{\sigma(wx+b), \quad w, b \in \mathbb{R}\}.$$

A classical result in Calculus states that if $\sigma \in C^\infty$ on any open interval and is not a polynomial thereon, then there exists a point $b^\star$ in that interval such that $\sigma^{(k)}(b^\star) \neq 0$ for all $k = 0, 1, 2, \cdots$.

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$$\frac{\sigma((w + h)x + b^\star) - \sigma(wx + b^\star)}{h} \in \mathcal{N}(\sigma; \mathbb{R}, \mathbb{R})$$

and so

$$\frac{d}{dw}\sigma(wx + b^\star)|_{w=0} = x\sigma'(b^\star) \in \overline{\mathcal{N}(\sigma; \mathbb{R}, \mathbb{R})}.$$

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$$\frac{d^k}{dw^k}\sigma\left(wx+b^{\star}\right)|_{w=0}=x^k\sigma^k(b^{\star})\in\overline{\mathcal{N}\left(\sigma;\mathbb{R},\mathbb{R}\right)}.$$

Since $\sigma^k(b^{\star})\neq 0$ for all k, then $\overline{\mathcal{N}\left(\sigma;\mathbb{R},\mathbb{R}\right)}$ contains all polynomials. By Weierstrass theorem, $\mathcal{N}\left(\sigma;\mathbb{R},\mathbb{R}\right)$ is dense in $C\left(K\right)$ for any compact set $K\subset\mathbb{R}$.

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

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Training error

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

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

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$$
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&+ \mathcal{E}_{\text{train, finalpos}} + \mathcal{E}_{\text{train, finalvel}},
\end{aligned}
$$

$$
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\mathcal{E}_{\text{train, int}} & = \left(\mathcal{L}_{\text{int}}\left(\boldsymbol{\theta}^*; \mathcal{T}_{\text{int}}\right)\right)^{1/2} \\
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\end{cases}
$$

Generalization error **for control and state**

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

Approximation theory and convergence analysis

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.

Recommendations

- **Data normalization.** It is important to ensure that the target output variables vary within a reasonable range. One way to achieve this is through non-dimensionalization of the PDE.

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  1. Compute

$$\begin{cases} \hat{\lambda}_{ic} = \frac{\|\nabla_\theta \mathcal{L}_{ic}(\theta)\| + \|\nabla_\theta \mathcal{L}_{bc}(\theta)\| + \|\nabla_\theta \mathcal{L}_r(\theta)\|}{\|\nabla_\theta \mathcal{L}_{ic}(\theta)\|} \\ \hat{\lambda}_{bc} = \frac{\|\nabla_\theta \mathcal{L}_{ic}(\theta)\| + \|\nabla_\theta \mathcal{L}_{bc}(\theta)\| + \|\nabla_\theta \mathcal{L}_r(\theta)\|}{\|\nabla_\theta \mathcal{L}_{bc}(\theta)\|} \\ \hat{\lambda}_r = \frac{\|\nabla_\theta \mathcal{L}_{ic}(\theta)\| + \|\nabla_\theta \mathcal{L}_{bc}(\theta)\| + \|\nabla_\theta \mathcal{L}_r(\theta)\|}{\|\nabla_\theta \mathcal{L}_r(\theta)\|} \end{cases} \tag{4}$$

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  2. Update the weights $\lambda = (\lambda_{ic}, \lambda_{bc}, \lambda_r)$ by using a moving average

$$\lambda_{\text{new}} = \alpha\lambda_{\text{old}} + (1-\alpha)\hat{\lambda}_{\text{new}}$$

Recommendations

- **Random weight factorization** may improve the performance of PINNs:

$$w^{(k,\ell)} = s^{(k,\ell)} v^{(k,\ell)},$$

with $s^{(k,\ell)}$ is a trainable scale factor assigned to each individual neuron.

S. Wang, et al..: *Random weight factorization improves the training of continuous neural representations.* **arXiv:2210.01274,** 2022.

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S. Wang, et al..: *Random weight factorization improves the training of continuous neural representations.* **arXiv:2210.01274,** 2022.

- **Optimization algorithm.** The Adaptive with Moment (Adam) algorithm is the most widely used to minimise the loss function. To speed up convergence near a local minimum, it is convenient to combine Adam (say, first 20000 iterations) with a quasi-Newton method like L-BFGS.

Shortcomings

- PINN has difficulty in approximating functions that have **steep gradients**. A Residual-based Adaptive Refinement algorithm has been proposed which add more residual points in the locations where the PDE residual is large.

Lu, L., Meng, X., Mao, Z. and Karniadakis, G.: *DeepXDE: A Deep Learning Library for Solving Differential Equations*, **SIAM Review, 63** (1), 208-228, 2021.

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- **MLPs are biased towards learning low frecuencies functions.** This can be mitigated by using a random Fourier feature embedding like

$$\gamma(x) = (\cos(Bx), \sin(Bx)),$$

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- **PINNs may violate temporal casuality** when solving time-dependent PDEs. We should partition the temporal domain into M equal sequential segments and introduce $\mathcal{L}_r^i(\theta)$ to denote the PDE residual loss within the i-th segment. The PDE residual becomes $\mathcal{L}_r(\theta) = \sum_{i=1}^{M} \lambda_i \mathcal{L}_r^i(\theta)$.

  S Wang, S Sankaran, H Wang, P Perdikaris:*An expert's guide to training physics-informed neural networks.* **ArXiv:2308.08468,** 2023.

Part III

Deep Operator Network (DeepONet)

Main objectives and references

Goals

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- Given two function spaces X and Y, and an operator

$$\mathcal{G} : X \to Y$$

the main goal is to learn (approximate) the operator $\mathcal{G}$ from a dataset.

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References

Lu, L., Jin, P., Pang, G., Zhang, Z., Karniadakis, G.E.:*Learning nonlinear operators via deeponet based on the universal approximation theorem of operators.* **Nature Machine Intelligence 3**(3), 218-229, 2021.

Lanthaler, S., Mishra, S., Karniadakis, G.E.:*Error estimates for DeepONets: a deep learning framework in infinite dimensions.* **Trans. Math. Appl. 6**(1), 1–144, 2022.

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

Problem setup

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: **approximate the controllabilty mapping**

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

where u is the **unique** control of minimal L^2-norm.

Problem setup

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

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

Goal: approximate the controllabilty mapping

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

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

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

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

Machine Learning setup

- **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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  $$\{(y_\ell^{\text{initial}}; t_\ell), \quad 1 \leq \ell \leq N\} \tag{5}$$

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- **Hypothesis space: the neural network**
  We will use the so-called **DeepONet**, which takes the form
  $$\mathcal{N}(\boldsymbol{\theta}; (y^{\text{initial}}(x_j); t)) := \sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma\left(\sum_{j=1}^{m} \xi_{ij}^k y^{\text{initial}}(x_j) + \theta_i^k\right) \cdot \sigma(w_k \cdot t + \eta_k) \tag{7}$$
  where $\boldsymbol{\theta} = (c_i^k, \xi_{ij}^k, \theta_i^k, w_k, \eta_k)$ is the set of parameters of the net.

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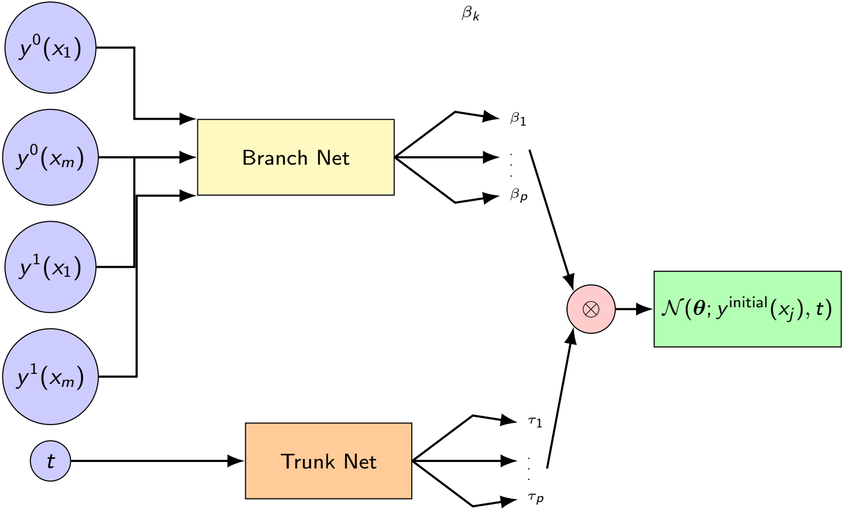
  where $\boldsymbol{\theta} = (c_i^k, \xi_{ij}^k, \theta_i^k, w_k, \eta_k)$ is the set of parameters of the net.
- **Loss function: Mean Squared Error (MSE)**
  $$\text{MSE}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{\ell=1}^{N} |\mathcal{N}(\boldsymbol{\theta}; (y_\ell^{\text{initial}}; t_\ell)) - u_\ell|^2 \tag{8}$$

DeepONet's architecture

$$\mathcal{N}(\boldsymbol{\theta}; (y^{\text{initial}}(x_j); t)) := \sum_{k=1}^{p} \underbrace{\sum_{i=1}^{n} c_i^k \sigma\left(\sum_{j=1}^{m} \xi_{ij}^k y^{\text{initial}}(x_j) + \theta_i^k\right)}_{\beta_k} \cdot \underbrace{\sigma(w_k \cdot t + \eta_k)}_{\tau_k}$$



Where does this architecture come from ?

Theorem (Universal Approximation Theorem for Functions)

Suppose that $K \in \mathbb{R}^d$ is compact, $U \subset C(K)$ is compact, and $\sigma \in$ is not a polynomial. Then, for any $\varepsilon > 0$ there exist a positive integer n, real numbers θ_i, $\omega_i \in \mathbb{R}^n$, independent of $f \in U$, and constants $c_i = c_i(f)$ depending on f, such that

$$|f(x) - \sum_{i=1}^{n} c_i \sigma(\omega_i \cdot x + \theta_i)| < \varepsilon$$

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Theorem (Universal Approximation Theorem for Functionals)

Suppose that σ *is not a polynomial,* X *is a Banach space,* $K \subset X$ *is a compact set,* V *is a compact set in* $C(K)$*, and* $f : V \to \mathbb{R}$ *is a continuous functional. Then for any* $\varepsilon > 0$*, there are a positive integer* n*,* m *sensor points* $x_1, x_2, \cdots, x_m \in K$*, and real constants* c_i, θ_i, ξ_{ij}*,* $1 \leq i \leq n$*,* $1 \leq j \leq m$*, such that*

$$|f(y) - \sum_{i=1}^{n} c_i \sigma\left(\sum_{j=1}^{m} \xi_{ij} y(x_j) + \theta_i\right)| < \varepsilon, \quad \text{for all } u \in V.$$

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Theorem (Universal Approximation Theorem for Operators)

Suppose that σ is not a polynomial, X is a Banach space, $K_1 \subset X$, $K_2 \subset \mathbb{R}^d$ are compact sets, V is a compact set in $C(K_1)$, and $\mathcal{G} : V \to C(K_2)$ is a continuous operator. Then for any $\varepsilon > 0$, there are a positive integers n, p, m sensor points $x_1, x_2, \cdots, x_m \in K_1$, and real constants $c_i^k, \theta_i^k, \xi_{ij}^k, \eta_k$ such that

$$|\mathcal{G}(y)(t) - \sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k y(x_j) + \theta_i^k \right) \sigma(\omega_k \cdot t + \zeta_k)| < \varepsilon, \quad \forall y \in V, t \in K_2$$

Chen, T., Chen, H.:*Universal approximation to nonlinear operators by neural networks with arbitrary activation functions and its application to dynamical systems.* **IEEE Transactions on Neural Networks 6**(4), 911-917, 1995.

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

$$\mu \sim \sum_{j=1}^{\infty} \sqrt{\lambda_j}\xi_j(\omega)\varphi_j(x) \tag{9}$$

We take $\xi_j \sim \mathcal{N}(0,1)$ i.i.d. standard Gaussian variables, and (λ_j, φ_j) the eigenpairs associated with squared exponential covariance function

$$C(x, x') = \sigma^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right). \tag{10}$$

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Thus, we truncate (9) and sample the Gaussian random variables. Remember that by Mercer's theorem $\{\varphi_j\}$ is an ortonormal basis of $L^2(0,1)$.

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

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

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
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Error analysis and the curse of dimensionality

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

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

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

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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

$$\mathcal{E}_{\text{optim}} := \|\mathcal{N}_M - \mathcal{N}_{\mathcal{T}}\|^{1/2}.$$

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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Some examples are:

- holomorphic mappings $[-1,1]^N \to V$, $y \mapsto \mathcal{G}(y)$ with V an arbitrary Banach space,

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- holomorphic mappings $[-1,1]^N \to V$, $y \mapsto \mathcal{G}(y)$ with V an arbitrary Banach space,
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  1. parametric elliptic PDEs: $\mathcal{G} : a \mapsto y$, where y solves

$$-\nabla \cdot (a\nabla y) = f$$

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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Error analysis and the curse of dimensionality

As for generalization error under suitable boundedness and Lipschitz continuity assumptions one gets

$$\mathcal{E}_{\text{gener}} \leq \frac{C}{\sqrt{N}} \left(1 + C d_\theta \log\left(CB\sqrt{N}\right)\right)^{2\kappa+\frac{1}{2}}$$

where N is the number of sampling functions, d_θ is the number of parameters of the DeepONet, and C, B and κ are suitable constants.

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Part IV

Numerical Implementation via DeepXDE

PINN. Experiment 1: the Laplace-Poisson equation

$$\begin{cases} -\Delta u(x) = -2d, & x \in D := (0,1)^d \\ u(x) = \sum_{k=1}^{d} x_k^2, & x \in \partial D \end{cases}$$

This problem has the exact solution

$$u_{\text{exact}}(x) = \sum_{k=1}^{d} x_k^2$$

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Python script is available at https://github.com/fperiago/deepcontrol

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Table: L^2- relative error $\frac{\| u_{\text{exact}} - u_{\text{PINN}} \|_{L^2(D)}}{\| u_{\text{exact}} \|_{L^2(D)}}$ for different values of the spatial dimension d and number of training points $N = N_{\text{interior}} + N_{\text{boundary}}$

	$N = 100 + 40$	$N = 1000 + 400$	$N = 10000 + 4000$
$d = 2$	9×10^{-4}	1.2×10^{-4}	7.5×10^{-5}
$d = 3$	1.2×10^{-3}	1.4×10^{-4}	1.3×10^{-3}
$d = 5$	2.5×10^{-2}	7.5×10^{-4}	1.9×10^{-4}
$d = 10$	2.2×10^{-1}	4.2×10^{-3}	2.2×10^{-3}
$d = 20$	3.1×10^{-1}	2.6×10^{-2}	2.5×10^{-3}

PINN. Experiment 1: the Laplace-Poisson equation

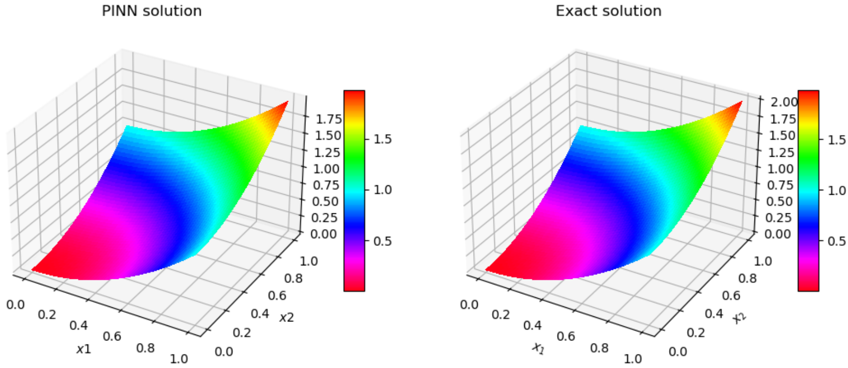

Figure: Experiment 1. Comparison between PINN (or predicted) solution u_{PINN} **(left)**, and exact solution u_{exact} **(right)**. Neural network composed of 3 hidden layers and 50 neurons in each layer. No regularization. Number of training points $N_{\text{interior}} = 100$, $N_{\text{boundary}} = 40$.

PINN. Experiment 2: exact 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 trough D'Alembert formula. Indeed, by considering the function

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

the explicit exact state is given by

$$y(x,t) = \frac{1}{2}\left(\tilde{y^0}(x-t) + \tilde{y^0}(x+t)\right), \quad 0 \le x \le 1,\ 0 \le t \le 2,$$

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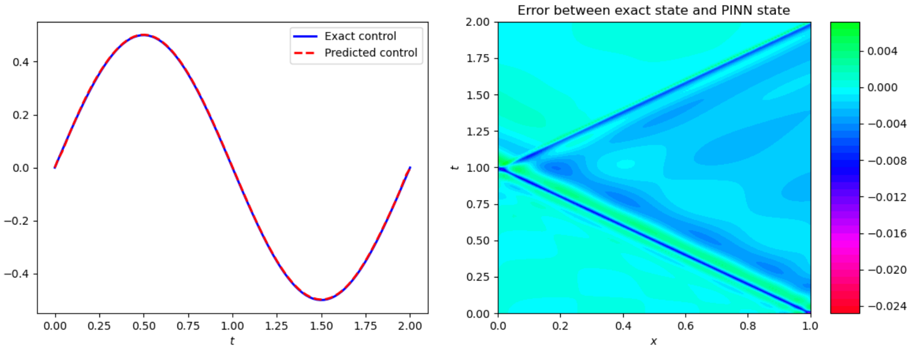

Figure: Experiment 1 (linear wave equation). Comparison between exact control $u(t)$ and PINN (or predicted) control $\hat{u}(t;\boldsymbol{\theta}^*)$ **(left)**, and error between exact state and PINN state, i.e. $y(x,t) - \hat{y}(x,t;\boldsymbol{\theta}^*)$ **(right)**. Neural network composed of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

DeepONet. Experiment 3: generation of training and test datasets

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

where u is the unique control of minimal L^2-norm of the system

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

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The **matrix of features** corresponds to initial conditions $(y^0(x), y^1(x))$ evaluated at a number of sensor points $x_j \in (0,1)$. It is computed by sampling a Gaussian random field

$$a(x,\omega) = \sum_{i=1}^{\infty} \sqrt{\lambda_i} e_i(x) \xi_i(\omega), \tag{12}$$

where ξ_i are iid standard Gaussian variables, and $\{\lambda_i, e_i(x)\}_{i=1}^{\infty}$ are the eigenvalues and normalized eigenfuncions of the operator

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

DeepONet. Experiment 3: generation of training and test datasets

The **vector of labels** corresponds to the exact control, which is given by

$$u(t) = \begin{cases} \frac{1}{2} y^0 (1-t) + \frac{1}{2} \int_{1-t}^{1} y^1(s)\, ds & 0 \le t \le 1 \\ \\ -\frac{1}{2} y^0 (t-1) + \frac{1}{2} \int_{t-1}^{1} y^1(s)\, ds & 1 \le t \le 2. \end{cases} \tag{13}$$

A data point is a triplet $((y^0, y^1), t, \mathcal{G}(y^0, y^1)(t))$.

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

DeepONet. Experiment 4: fitting the deeponet model

The implementation in DeepXDE is as follows:

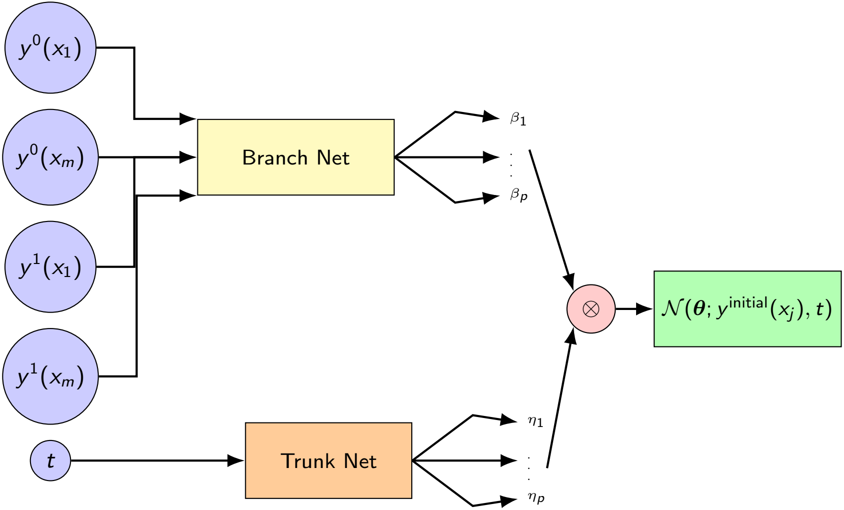
```
    X_train = (X_train[:, :-1], X_train[:, -1:])
    X_test = (X_test[:, :-1], X_test[:, -1:])

    data = dde.data.Triple(
    X_train=X_train, y_train=y_train, X_test=X_test, y_test=
        y_test
    )
```

Lu, L., Jin, P., Pang, G., Zhang, Z., Karniadakis, G.E.:*Learning nonlinear operators via deeponet based on the universal approximation theorem of operators.* **Nature Machine Intelligence 3**(3), 218-229, 2021.

DeepONet. Experiment 4: fitting the deeponet model

Next, we select the architecture of the DeepONet



DeepONet. Experiment 4: fitting the deeponet model

The implementation in DeepXDE is as follows:

```python
m = X_train_input_dimension  # inferred from training data

dim_t = 1  # input dimension of the trunk

p = 10  # output dimension of the branch and trunk nets

net = dde.nn.DeepONet(
[m, 40, p],         # dimensions of the branch net
[dim_t, 40, p],     # dimensions of the trunk net
"relu",             # activation function
"Glorot normal",    # initialization of parameters
)

model = dde.Model(data, net)

model.compile("adam", lr=0.001)

losshistory, train_state = model.train(iterations=ITERATIONS)

dde.saveplot(losshistory, train_state, issave=True, isplot=True)
```

DeepONet. Experiment 4: Smooth initial conditions

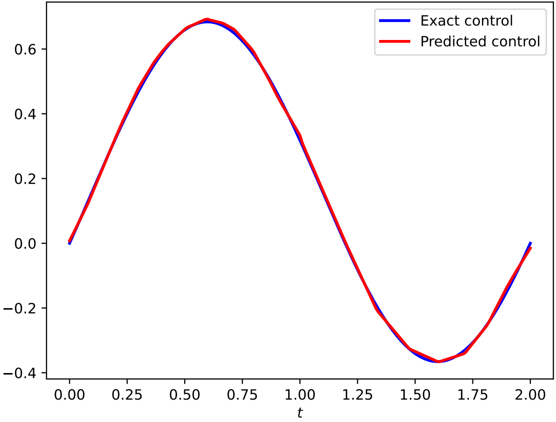


Figure: Experiment 4: wave equation. Exact versus predicted solutions for THE smooth initial conditions $y^0(x) = y^1(x) = \sin(\pi x)$. $n_{functions} = 10^4$, $(\ell_0, \ell_1) = (0.25, 0.125)$, $n_{sensors} = 101$, $p = 40$. Relative error $\approx 1\%$.

DeepONet. Experiment 4: Unsmooth initial conditions

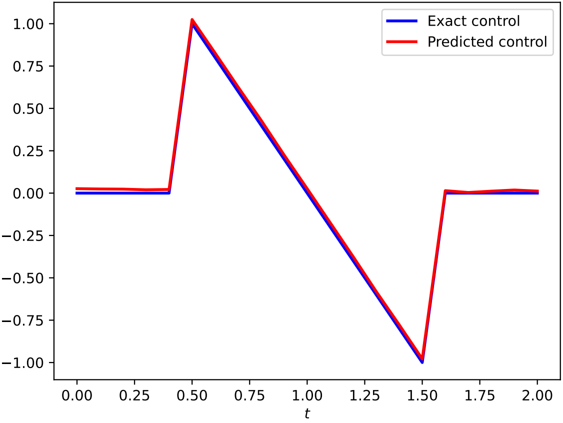


Figure: Experiment 4: wave equation. Exact versus predicted solutions for the unsmooth initial conditions $y^0(x) = \begin{cases} 4x, & 0 \leq x \leq 0.5 \\ 0, & 0.5 < x \leq 1 \end{cases}, \quad y^1(x) = 0.$ $n_{functions} = 10^4$, $(\ell_0, \ell_1) = (0.03125, 0.03125)$, $p = 100$. $n_{sensors} = 11$. Relative error $\approx 4\%$.

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Thank you for your attention !