A first step towards numerical approximation of controllability problems via Deep- Learning-based methods

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Goals, outline and references

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- Provide error estimates for the so-called generalization error

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References

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A toy model: controllability of the linear wave equation

The exact controllability problem: given initial data $(y^0(x), y^1(x))$ and a positive time $T > 0$ find a boundary control $u(t)$ such that the solution $y(x,t)$ of the system

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

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For $T = 2/c$ this problem has the explicit solution

$$u(t) = \begin{cases} \frac{1}{2} y^0(1-ct) + \frac{1}{2c} \int_{1-ct}^{1} y^1(s)\, ds & 0 \le t \le 1/c \\ \\ -\frac{1}{2} y^0(ct-1) + \frac{1}{2c} \int_{ct-1}^{1} y^1(s)\, ds & 1/c \le t \le 2/c \end{cases} \tag{3}$$

Numerical approximation of the control via PINNs

Main steps of the PINNs algorithm

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   From the training process, optimal parameters $\boldsymbol{\theta}$ defining the neural network $\hat{y}(x, t; \boldsymbol{\theta})$ are computed and eventually are used to get predictions about the state $y(x, t)$ and the control $u(t)$, which is approximated as the trace of $\hat{y}(x, t; \boldsymbol{\theta})$ on the boundary $x = 1$, i.e., the surrogate control $\hat{u}(t; \boldsymbol{\theta}) = \hat{y}(1, t; \boldsymbol{\theta})$

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Step 1: Neural network.

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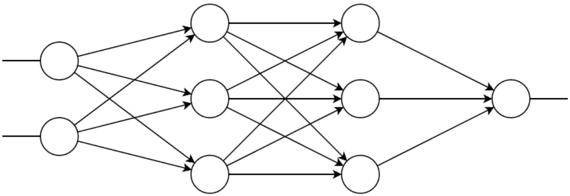
Step 1: Neural network. We consider a Multilayer Perceptron (MLP) with two input canals $\boldsymbol{x} = (x, t) \in \mathbb{R}^2$ and an scalar output $\hat{y}$. Precisely, $\hat{y}\,(x, t; \boldsymbol{\theta})$ is constructed as

$$\begin{cases} \text{input layer:} & \mathcal{N}^0(\boldsymbol{x}) = \boldsymbol{x} = (x, t) \in \mathbb{R}^2 \\ \text{hidden layers:} & \mathcal{N}^\ell(\boldsymbol{x}) = \sigma\left(\boldsymbol{W}^\ell \mathcal{N}^{\ell-1}(\boldsymbol{x}) + \boldsymbol{b}^\ell\right) \in \mathbb{R}^{N_\ell} \\ \text{output layer:} & \hat{y}\,(\boldsymbol{x}; \boldsymbol{\theta}) = \mathcal{N}^L(\boldsymbol{x}) = \boldsymbol{W}^L \mathcal{N}^{L-1}(\boldsymbol{x}) + \boldsymbol{b}^L \in \mathbb{R} \end{cases} \tag{4}$$

where

- $\mathcal{N}^\ell(\boldsymbol{x}) : \mathbb{R}^{d_{in}} \to \mathbb{R}^{d_{out}}$ 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 a smooth activation function, e.g. the hyperbolic tangent $\sigma(s) = \tanh(s)$.



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Step 2: Training dataset.

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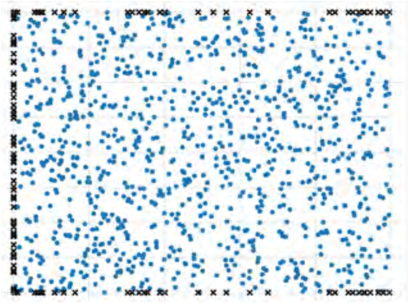

Step 3: Loss function.

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Step 3: Loss function. It is composed of the following six terms:

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

Numerical approximation of the control via PINNs: the details

Step 4: Training process. The final step at the PINN algorithm amounts to minimize the loss function

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta};\mathcal{T}) \quad &= \mathcal{L}_{\text{int}}(\boldsymbol{\theta};\mathcal{T}_{\text{int}}) \\ &+\mathcal{L}_{x=0}(\boldsymbol{\theta};\mathcal{T}_{x=0}) \\ &+\mathcal{L}^{\text{pos}}_{t=0}(\boldsymbol{\theta};\mathcal{T}_{t=0}) + \mathcal{L}^{\text{vel}}_{t=0}(\boldsymbol{\theta};\mathcal{T}_{t=0}) \\ &+\mathcal{L}^{\text{pos}}_{t=T}(\boldsymbol{\theta};\mathcal{T}_{t=T}) + \mathcal{L}^{\text{vel}}_{t=T}(\boldsymbol{\theta};\mathcal{T}_{t=T}).\end{aligned} \tag{5}$$

i.e., we compute

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta};\mathcal{T}). \tag{6}$$

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The descent algorithm **ADAM** (Adaptive with Moment) is chosen for numerical implementation. Automatic Differentation **AD**, which is included in TensorFlow, is used for computation of gradients.

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The descent algorithm **ADAM** (Adaptive with Moment) is chosen for numerical implementation. Automatic Differentation **AD**, which is included in TensorFlow, is used for computation of gradients.
The approximation $\hat{u}(t;\boldsymbol{\theta}^*)$ of the control $u(t)$ is then obtained as the restriction of $\hat{y}(x,t;\boldsymbol{\theta}^*)$ to the boundary $x=1$, i.e.

$$\hat{u}(t;\boldsymbol{\theta}^*) = \hat{y}(1,t;\boldsymbol{\theta}^*), \quad 0 \le t \le T. \tag{7}$$

Error estimates for generalization error

Generalization error for the control

$$\mathcal{E}_{\text{gener}}(u) := \|u - \hat{u}\|_{L^2(0,T)}, \tag{8}$$

where $u = u(t)$ is the exact control of the continuous problem and $\hat{u} = \hat{u}(t; \boldsymbol{\theta}^*)$ is its numerical approximation via PINN algo.

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Our goal is to get estimations for generalization error in terms of error estimates for quadrature and the so-called training error.
Quadrature errors:

$$|\overline{f} - \overline{f}_N| \leq C_q(d) N^{-\alpha}, \quad \alpha > 0, \tag{9}$$

where

$$\overline{f} := \int_{\mathcal{D}} f(x)\, dx, \quad \overline{f}_N := \sum_{j=1}^{N} w_j f(x_j)$$

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Training error: $\mathcal{E}_{\text{train}} := \mathcal{L}(\boldsymbol{\theta}^*; \mathcal{T})$

$$\begin{cases} \mathcal{E}_{\text{train, int}} & = \mathcal{L}_{\text{int}}(\boldsymbol{\theta}^*; \mathcal{T}_{\text{int}}) \\ \mathcal{E}_{\text{train, boundary}} & = \mathcal{L}_{x=0}(\boldsymbol{\theta}^*; \mathcal{T}_{x=0}) \\ \mathcal{E}_{\text{train, initialpos}} & = \mathcal{L}^{\text{pos}}_{t=0}(\boldsymbol{\theta}^*; \mathcal{T}_{t=0}) \\ \mathcal{E}_{\text{train, initialvel}} & = \mathcal{L}^{\text{vel}}_{t=0}(\boldsymbol{\theta}^*; \mathcal{T}_{t=0}) \\ \mathcal{E}_{\text{train, finalpos}} & = \mathcal{L}^{\text{pos}}_{t=T}(\boldsymbol{\theta}^*; \mathcal{T}_{t=T}) \\ \mathcal{E}_{\text{train, finalvel}} & = \mathcal{L}^{\text{vel}}_{t=T}(\boldsymbol{\theta}^*; \mathcal{T}_{t=T}). \end{cases} \tag{10}$$

Error estimates for generalization error

Theorem

Let $y = y(x,t) \in C^k\left(\overline{Q_T}\right)$, $k \geq 2$, *be the unique classical solution of* (1)-(2) *and let* $\hat{y} = \hat{y}(x,t;\boldsymbol{\theta}^*)$ *its PINN approximation. Let* $u = u(t)$ *and* $\hat{u} = \hat{u}\left(t;\boldsymbol{\theta}^*\right)$ *be the exact control of the continuous system* (1)-(2) *and its PINN approximation, respectively. Then, the following estimate for generalization error holds*

$$\begin{aligned}
\mathcal{E}_{gener}(u) \quad &\lesssim \mathcal{E}_{train,\ int} + CN_{int}^{-\alpha/2} \\
&+\mathcal{E}_{train,\ boundary} + CN_{b}^{-\alpha/2} \\
&+\mathcal{E}_{train,\ initialpos} + CN_{0}^{-\alpha/2} \\
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Main ingredients in the proof are observability inequalities and energy estimates

Error estimates for generalization error

Lemma (E. Fernández-Cara and E. Zuazua)

Let $T \geq 2$. Given initial and final conditions $(z_0^0, z_0^1), (z_T^0, z_T^1) \in L^2(0,1) \times H^{-1}(0,1)$, there exists a control function $v \in L^2(0,T)$ such that the solution $z(x,t)$ of the system

$$\begin{cases} z_{tt} = z_{xx}, & \text{in } Q_T \\ z(x,0) = z_0^0(x), & \text{in } (0,1) \\ z_t(x,0) = z_0^1(x) & \text{in } (0,1) \\ z(0,t) = 0, \quad z(1,t) = v(t) & \text{on } (0,T) \end{cases} \tag{12}$$

satisfies

$$z(x,T) = z_T^0(x), \quad z_t(x,T) = z_T^1(x,T), \quad x \in (0,1). \tag{13}$$

Moreover,

$$\|v\|_{L^2(0,T)} \leq C\left(\|z_0^0\|_{L^2(0,1)} + \|z_0^1\|_{H^{-1}(0,1)} + \|z_T^0\|_{L^2(0,1)} + \|z_T^1\|_{H^{-1}(0,1)}\right), \tag{14}$$

for a positive constant $C = C(T)$, which does not depend on the initial and final data.

Error estimates for generalization error

Lemma

Consider the non-homogeneous system

$$\begin{cases} z_{tt} = z_{xx} + f(x,t), & \text{in } Q_T \\ z(x,0) = z_0^0(x), & \text{in } (0,1) \\ z_t(x,0) = z_0^1(x) & \text{in } (0,1) \\ z(0,t) = g_0(t), \quad z(1,t) = g_1(t) & \text{on } (0,T) \end{cases}$$

Then, there exists a positive constant C such that

$$\|z\|_{C\left(0,T;L^2(0,1)\right)} + \|z_t\|_{C\left(0,T;H^{-1}(0,1)\right)} \\ \leq C\left(\|z_0^0\|_{L^2(0,1)} + \|z_0^1\|_{H^{-1}(0,1)} + \|g_0\|_{L^2(0,T)} + \|g_1\|_{L^2(0,T)} + \|f\|_{L^2\left(0,T;L^2(0,1)\right)}\right)$$

Proof of theorem on generalization error.

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Proof of theorem on generalization error.

Let $\overline{y} = y - \hat{y}$ and $\overline{u} = u - \hat{u}$ be the error in the state and control variables, respectively.By linearity, $\overline{y}$ solves

$$\begin{cases} \overline{y}_{tt} - \overline{y}_{xx} = \hat{y}_{tt} - \hat{y}_{xx}, & \text{in } Q_T \\ \overline{y}(x,0) = y^0(x) - \hat{y}(x,0), & \text{in } (0,1) \\ \overline{y}_t(x,0) = y^1(x) - \hat{y}_t(x,0) & \text{in } (0,1) \\ \overline{y}(x,T) = \hat{y}(x,T), & \text{in } (0,1) \\ \overline{y}_t(x,T) = \hat{y}_t(x,T) & \text{in } (0,1) \\ \overline{y}(0,t) = \hat{y}(0,t), \quad \overline{y}(1,t) = u(t) - \hat{y}(1,t) & \text{on } (0,T). \end{cases} \tag{15}$$

Error estimates for generalization error

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$\overline{y}(x,t;\boldsymbol{\theta})$ is decomposed as $\overline{y} = \overline{y}^1 + \overline{y}^2$, where

$$\begin{cases} \overline{y}^1_{tt} - \overline{y}^1_{xx} = 0, & \text{in } Q_T \\ \overline{y}^1(x,0) = y^0(x) - \hat{y}(x,0), & \text{in } (0,1) \\ \overline{y}^1_t(x,0) = y^1(x) - \hat{y}_t(x,0) & \text{in } (0,1) \\ \overline{y}^1(0,t) = 0, \quad \overline{y}^1(1,t) = u(t) - \hat{y}(1,t) & \text{on } (0,T). \end{cases} \tag{16}$$

$$\begin{cases} \overline{y}^2_{tt} - \overline{y}^2_{xx} = \hat{y}_{tt} - \hat{y}_{xx}, & \text{in } Q_T \\ \overline{y}^2(x,0) = 0, \quad \overline{y}^2_t(x,0) = 0 & \text{in } (0,1) \\ \overline{y}^2(x,T) = \hat{y}(x,T) - \overline{y}^1(x,T), & \text{in } (0,1) \\ \overline{y}^2_t(x,T) = \hat{y}_t(x,T) - \overline{y}^1_t(x,T), & \text{in } (0,1) \\ \overline{y}^2(0,t) = \hat{y}(0,t), \quad \overline{y}^2(1,t) = 0 & \text{on } (0,T). \end{cases} \tag{17}$$

Error estimates for generalization error

Proof of theorem on generalization error.

By applying the observability inequality to system (16) and the energy estimate to (17),

$$\|u - \hat{u}\|_{L^2(0,T)}$$

$$\lesssim \|y^0 - \hat{y}(\cdot,0)\|_{L^2(0,1)} + \|y^1 - \hat{y}_t(\cdot,0)\|_{H^{-1}(0,1)} + \|\overline{y}^1(\cdot,T)\|_{L^2(0,1)} + \|\overline{y}^1_t(\cdot,T)\|_{H^{-1}(0,1)}$$

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$$\lesssim \|y^0-\hat{y}(\cdot,0)\|_{L^2(0,1)}+\|y^1-\hat{y}_t(\cdot,0)\|_{L^2(0,1)}+\|\hat{y}(\cdot,T)\|_{L^2(0,1)}+\|\hat{y}_t(\cdot,T)\|_{L^2(0,1)}$$

$$+\|\overline{y}^2(\cdot,T)\|_{L^2(0,1)}+\|\overline{y}_t^2(\cdot,T)\|_{H^{-1}(0,1)}$$

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$$\begin{aligned}
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&\lesssim \|y^0-\hat{y}(\cdot,0)\|_{L^2(0,1)}+\|y^1-\hat{y}_t(\cdot,0)\|_{L^2(0,1)}+\|\hat{y}(\cdot,T)\|_{L^2(0,1)}+\|\hat{y}_t(\cdot,T)\|_{L^2(0,1)}\\
&+\|\overline{y}^2(\cdot,T)\|_{L^2(0,1)}+\|\overline{y}^2_t(\cdot,T)\|_{H^{-1}(0,1)}\\
&\lesssim \|y^0-\hat{y}(\cdot,0)\|_{L^2(0,1)}+\|y^1-\hat{y}_t(\cdot,0)\|_{L^2(0,1)}+\|\hat{y}(\cdot,T)\|_{L^2(0,1)}+\|\hat{y}_t(\cdot,T)\|_{L^2(0,1)}\\
&+\|\hat{y}\,(0,\cdot)\,\|_{L^2(0,T)}+\|\hat{y}_{tt}-\hat{y}_{xx}\|_{L^2(0,T;L^2(0,1))}.
\end{aligned} \tag{18}$$

The result then follows by applying estimates error for quadrature (9).

A numerical experiment (preliminary results)

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

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Numerical implentation via DeepXDE Python library

- Multilayer perceptron with 4 hidden layers and 50 neurons in each layer
- Activation function: tanh
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Table: Summary of results for training errors and for 500 interior points and 50 boundary points.

$\|\hat{y}_{tt} - \hat{y}_{xx}\|$	$\|\hat{y}(0,\cdot)\|$	$\|y^0 - \hat{y}(\cdot,0)\|$	$\|y^1 - \hat{y}_t(\cdot,0)\|$	$\|\hat{y}(\cdot,T)\|$	$\|\hat{y}_t(\cdot,T)\|$
8.8×10^{-6}	2.1×10^{-6}	1.1×10^{-6}	5.7×10^{-9}	3.4×10^{-8}	7.3×10^{-8}

A numerical experiment (preliminary results)

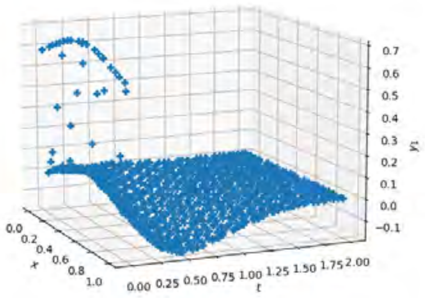

Figure: Predicted solution.

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.... Muchas gracias ....