Physics-Informed Neural Networks for Nonsmooth PDE-Constrained Optimization Problems

Yongcun Song

Chair for Dynamics, Control, Machine Learning and Numerics-Alexander von Humboldt-Professorship
Department of Mathematics, Friedrich-Alexander-Universität Erlangen-Nürnberg

Background and Motivation

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- A given objective functional has to be minimized subject to a PDE or a system of coupled PDEs, usually with other additional constraints.
- PDE-constrained optimization problems arise.

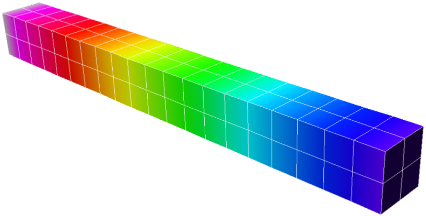

Figure 1: Control the heat distribution of a metal bar

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  - the constraints $u \in U_{ad}$ and $y \in Y_{ad}$ describe some physical restrictions and realistic requirements.

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- A parabolic sparse optimal control problem:

$$\min_{y,u\in L^2(Q)} \mathcal{J}(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2(Q)} + \rho\|u\|_{L^1(Q)} + I_{U_{ad}}(u),$$

subject to

$$\frac{\partial y}{\partial t} - \nu\Delta y + c_0 y = u + f \text{ in } \Omega \times (0,T), \; y = 0 \text{ on } \partial\Omega \times (0,T), \; y(0) = \varphi.$$

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  - Above, Ω is a bounded domain in $\mathbb{R}^d$ with $d \geq 1$ and $\partial\Omega$ is its boundary; $Q = \Omega \times (0,T)$ with $0 < T < +\infty$; $y_d \in L^2(Q)$ and $\phi \in L^2(\Omega), f \in L^2(Q)$ are given.
  - The regularization parameters $\alpha \geq 0$, $\rho > 0$ and the coefficients $\nu > 0$, $c_0 \geq 0$ are constant.
  - $I_{U_{ad}}(\cdot)$ is the indicator function of $U_{ad} := \{u \in L^2(\Omega) | a \leq u(x,t) \leq b, \text{ a.e. in } Q\}$, where $a, b \in L^2(\Omega)$ with $a < 0 < b$ almost everywhere.

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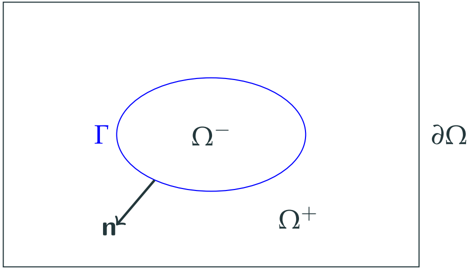

Figure 2: The geometry of an interface problem: an illustration

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- An elliptic interface optimal control problem:

$$\min_{y\in L^2(\Omega),u\in L^2(\Omega)} J(y,u) := \frac{1}{2}\|y-y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)},$$

subject to

$$\begin{cases} -\nabla\cdot(\beta\nabla y) = u + f & \text{in } \Omega\backslash\Gamma, \\ [y]_\Gamma = g_0,\ [\beta\partial_{\boldsymbol{n}} y]_\Gamma = g_1 & \text{on } \Gamma, \\ y = h_0 & \text{on } \partial\Omega, \end{cases}$$

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  - The jump discontinuity across Γ: $[y]_\Gamma(x) := \lim_{\tilde{x}\to x \text{ in } \Omega^+} y(\tilde{x}) - \lim_{\tilde{x}\to x \text{ in } \Omega^-} y(\tilde{x}), \forall x\in\Gamma.$

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- The operator $\partial_{\boldsymbol{n}}$ stands for the normal derivative on Γ, i.e. $\partial_{\boldsymbol{n}} y(x) = \boldsymbol{n}\cdot\nabla y(x)$ with $\boldsymbol{n}\in\mathbb{R}^d$ the outward unit normal vector of Γ. In particular, we have

$$[\beta\partial_{\boldsymbol{n}} y]_\Gamma(x) := \boldsymbol{n}\cdot(\beta^+ \lim_{\tilde{x}\to x \text{ in } \Omega^+} \nabla y(\tilde{x}) - \beta^- \lim_{\tilde{x}\to x \text{ in } \Omega^-} \nabla y(\tilde{x})), \quad \forall x\in\Gamma.$$

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- Moreover, these methods are strongly problem-dependent, e.g., different types of PDEs entail different tailored numerical discretization schemes.

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  - Operator learning methods: DeepONets [Lu, Jin, Pang, Zhang, and Karniadakis, 2021], Fourier Neural Operator, Graph Neural Operator, [Li, Kovachki, Azizzadenesheli, Liu, Bhattacharya, Stuart, and Anandkumar,2020] and Laplace Neural Operator [Cao, Goswami, and Karniadakis, 2023], etc.
  - ... ...

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- Given an input point in the domain, PINNs produce an approximate solution in that point of a PDE after training.

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where $\mathcal{L}_i(\boldsymbol{\theta}, \mathcal{T}_i) = \frac{1}{|\mathcal{T}_i|} \sum_{x \in \mathcal{T}_i} \|\mathcal{E}(\hat{y}(x; \boldsymbol{\theta}), u(x))\|^2$, $\mathcal{L}_b(\boldsymbol{\theta}, \mathcal{T}_b) = \frac{1}{|\mathcal{T}_b|} \sum_{x \in \mathcal{T}_b} \|\mathcal{B}(\hat{y}(x; \boldsymbol{\theta}), u(x))\|^2$, and $w_i > 0$ and $w_b > 0$ are the weights.

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4. Train the neural network $\hat{y}(x;\boldsymbol{\theta})$ to find the optimal parameters $\boldsymbol{\theta}^*$ by minimizing the loss function $\mathcal{L}_{PDE}(\boldsymbol{\theta},\mathcal{T})$. At the end of the training procedure, the trained neural network $\hat{y}(x,\boldsymbol{\theta}^*)$ approximately solves the PDE.

PINNs

- Pros of PINNs:
  - little or even no labeled data is required
  - easy to implement
  - mesh-free
  - flexible to different problem settings

PINNs for Smooth PDE-Constrained Optimization

- PINNs for smooth PDE-Constrained Optimization, see e.g., [Mowlavi and Nabi, 2023; Barry-Straume, Sarshar, Popov, and Sandu, 2022; Jin, Sau, Yin, and Zhou, 2023]

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- Consider the smooth PDE-constrained optimization problems modeled by

$$\min \mathcal{J}(u, y), \quad \text{s.t.} \quad e(u, y) = 0.$$

- Let $\hat{y}(x; \boldsymbol{\theta}_y)$ parameterized by $\boldsymbol{\theta}_y$ and $\hat{u}(x; \boldsymbol{\theta}_u)$ parameterized by $\boldsymbol{\theta}_u$ be two neural networks to approximate y and u, respectively.
- Specify the residual points $\mathcal{T} \subset \Omega \cup \partial\Omega$ and a loss function by summing the PDE's residual and the objective functional:

$$\mathcal{L}_{total}(\boldsymbol{\theta}_y, \boldsymbol{\theta}_u, \mathcal{T}) = w_o \mathcal{J}(\boldsymbol{\theta}_y, \boldsymbol{\theta}_u, \mathcal{T}) + w_p \mathcal{L}_{PDE}(\boldsymbol{\theta}_y, \boldsymbol{\theta}_u, \mathcal{T}),$$

  where w_o and w_p are the weights.
- Train the neural networks $\hat{y}(x; \boldsymbol{\theta}_y)$ and $\hat{u}(x; \boldsymbol{\theta}_u)$ by minimizing the loss function $\mathcal{L}_{total}(\boldsymbol{\theta}_y, \boldsymbol{\theta}_u, \mathcal{T})$. At the end of the training procedure, we obtain the solution $\hat{y}(x, \boldsymbol{\theta}_y^*)$ and $\hat{u}(x, \boldsymbol{\theta}_u^*)$

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- For the parabolic sparse optimal control problem:
    - the nonsmooth term $\rho\|\hat{u}(x;\boldsymbol{\theta}_u)\|_{L^1(Q)} + I_{U_{ad}}(\hat{u}(x;\boldsymbol{\theta}_u))$ appears in the loss function.

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    - commonly used neural network training technologies (e.g., back-propagation and stochastic gradient methods) cannot be applied directly.
- For the elliptic interface optimal control problem:
    - the discontinuity or nonsmoothness of y cannot be well captured by the neural network $\hat{y}(x;\boldsymbol{\theta}_y)$ because the activation functions used in a DNN are in general smooth (e.g., the sigmoid function) or at least continuous (e.g., the rectified linear unit (ReLU) function).

The ADMM-PINNs for Parabolic Sparse Optimal Control Problems

Parabolic Sparse Optimal Control: Revisit

- We first recall the parabolic sparse optimal control problem under investigation:

$$\min_{y,u\in L^2(Q)} \frac{1}{2}\|y-y_d\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2(Q)} + \rho\|u\|_{L^1(Q)} + I_{U_{ad}}(u),$$

subject to

$$\frac{\partial y}{\partial t} - \nu\Delta y + c_0 y = u + f \text{ in } \Omega\times(0,T),\ y=0 \text{ on } \partial\Omega\times(0,T),\ y(0)=\varphi.$$

  - Above, Ω is a bounded domain in $\mathbb{R}^d$ with $d\geq 1$ and $\partial\Omega$ is its boundary; $Q=\Omega\times(0,T)$ with $0<T<+\infty$; $y_d\in L^2(Q)$ and $\phi\in L^2(\Omega), f\in L^2(Q)$ are given.
  - The regularization parameters $\alpha>0$, $\rho>0$ and the coefficients $\nu>0$, $c_0\leq 0$ are assumed to be constant.
  - $I_{U_{ad}}(\cdot)$ the indicator function of $U_{ad}:=\{u\in L^\infty(\Omega)|a\leq u(x,t)\leq b,\ \text{a.e. in } Q\}\subset L^2(Q)$, where $a,b\in L^2(\Omega)$ with $a<0<b$ almost everywhere.

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- Operator splitting.
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- The nonsmooth PDE-constrained optimization problem is decoupled into two simpler subproblems:
  - one smooth PDE-constrained optimization which can be efficiently solved by PINNs
  - the other is a simple nonsmooth optimization problem which usually has a closed-form solution or can be efficiently solved by various standard optimization algorithms or pre-trained neural networks.

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$$\min_{u,z \in L^2(Q)} \frac{1}{2}\|y(u) - y_d\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2(Q)} + \rho\|z\|_{L^1(Q)} + I_{U_{ad}}(z), \quad \text{s.t.} \qquad u = z.$$

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- The augmented Lagrangian functional reads as

$$L^{SC}_{\beta}(u, z; \lambda) = \frac{1}{2}\|y(u) - y_d\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2(Q)} - (\lambda, u - z)_{L^2(Q)} + \frac{\beta}{2}\|u - z\|^2_{L^2(Q)},$$

where $\lambda \in L^2(Q)$ is the Lagrange multiplier associated with $u = z$ and $\beta > 0$ is a penalty parameter.

ADMM-Cont'd

- The ADMM iterative scheme:

$$\begin{cases} u^{k+1} = \arg\min_{u \in L^2(Q)} L_\beta^{SC}(u, z^k; \lambda^k), \\ z^{k+1} = \arg\min_{z \in L^2(Q)} L_\beta^{SC}(u^{k+1}, z; \lambda^k), \\ \lambda^{k+1} = \lambda^k - \beta(u^{k+1} - z^{k+1}). \end{cases}$$

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- The z-subproblem is

$$z^{k+1} = \arg\min_{z \in L^2(Q)} I_{U_{ad}}(z) + \rho\|z\|_{L^1(Q)} - (\lambda^k, u^{k+1} - z)_{L^2(Q)} + \frac{\beta}{2}\|u^{k+1} - z\|^2_{L^2(Q)}.$$

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- The solution z^{k+1} can be computed by

$$z^{k+1} = \mathbb{P}_{U_{ad}}\left(\mathbb{S}_{\frac{\rho}{\beta}}\left(u^{k+1} - \frac{\lambda^k}{\beta}\right)\right),$$

where $\mathbb{S}_\zeta$ is the Shrinkage operator: $\mathbb{S}_\zeta(v)(x) = \mathrm{sgn}(v(x))(|v(x)| - \zeta)_+, \forall\, \zeta > 0$.

PINNs for the u-Subproblem

- The u-subproblem can be reformulated as

$$\min_{y,u} \mathcal{J}_{SC}^{k}(y,u) := \frac{1}{2}\|y(u) - y_d\|_{L^2(Q)}^2 + \frac{\alpha}{2}\|u\|_{L^2(Q)}^2 - (\lambda^k, u - z^k)_{L^2(Q)} + \frac{\beta}{2}\|u - z^k\|_{L^2(Q)}^2$$

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- The first-order optimality system reads as

$$\begin{cases} p + (\alpha+\beta)u - \lambda^k - \beta z^k = 0, \\ \dfrac{\partial y}{\partial t} - \nu\Delta y + c_0 y = u + f \text{ in } \Omega\times(0,T), \quad y = 0 \text{ on } \partial\Omega\times(0,T), \quad y(0) = \varphi, \\ -\dfrac{\partial p}{\partial t} - \nu\Delta p + c_0 p = y - y_d \text{ in } \Omega\times(0,T), \quad p = 0 \text{ on } \partial\Omega\times(0,T), \quad p(T) = 0, \end{cases}$$

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  where p is the corresponding adjoint variable.
- Eliminate the variable u, and then construct two neural networks $\hat{y}(x;\boldsymbol{\theta}_y)$ parameterized by $\boldsymbol{\theta}_y$ and $\hat{p}(x;\boldsymbol{\theta}_p)$ parameterized by $\boldsymbol{\theta}_p$ to approximate y and p, respectively.

PINNs for the u-Subproblem-Cont'd

- Choose residual points $\mathcal{T}_i \subset \Omega \times (0, T)$, $\mathcal{T}_{b_1} \subset \partial\Omega \times (0, T)$, and $\mathcal{T}_{b_2} \subset \Omega$.
- Specify a loss function by summing the residuals of the first-order optimality system

$$
\begin{aligned}
\mathcal{L}_{OS}(\boldsymbol{\theta}_y, \boldsymbol{\theta}_p) = w_y\Big(&\frac{w_i}{|\mathcal{T}_i|}\sum_{\{x,t\}\in\mathcal{T}_i}\Big|\frac{\partial \hat{y}(x,t;\boldsymbol{\theta}_y)}{\partial t} - \nu\frac{\partial^2 \hat{y}(x,t;\boldsymbol{\theta}_y)}{\partial x^2} + c_0\hat{y}(x,t;\boldsymbol{\theta}_y) \\
&- \frac{1}{\alpha+\beta}\big(-\hat{p}(x,t;\boldsymbol{\theta}_p) + \lambda^k(x,t) + \beta z^k(x,t)\big) - f(x,t)\Big|^2 \\
&+ \frac{w_{b_1}}{|\mathcal{T}_{b_1}|}\sum_{\{x,t\}\in\mathcal{T}_{b_1}}|\hat{y}(x,t;\boldsymbol{\theta}_y)|^2 + \frac{w_{b_2}}{|\mathcal{T}_{b_2}|}\sum_{x\in\mathcal{T}_{b_2}}|\hat{y}(x,0;\boldsymbol{\theta}_y) - \varphi(x)|^2\Big) \\
+ w_p\Big(&\frac{w_i}{|\mathcal{T}_i|}\sum_{\{x,t\}\in\mathcal{T}_i}\Big|-\frac{\partial \hat{p}(x,t;\boldsymbol{\theta}_p)}{\partial t} - \nu\Delta\hat{p}(x,t;\boldsymbol{\theta}_p) + c_0\hat{p}(x,t;\boldsymbol{\theta}_p) - \hat{y}(x,t;\boldsymbol{\theta}_y) + y_d(x,t)\Big|^2 \\
&+ \frac{w_{b_1}}{|\mathcal{T}_{b_1}|}\sum_{\{x,t\}\in\mathcal{T}_{b_1}}|\hat{p}(x,t;\boldsymbol{\theta}_p)|^2 + \frac{w_{b_2}}{|\mathcal{T}_{b_2}|}\sum_{x\in\mathcal{T}_{b_2}}|\hat{p}(x,0;\boldsymbol{\theta}_p)|^2\Big)
\end{aligned}
$$

- Train the neural networks to update the parameters $\boldsymbol{\theta}_y^{k+1}$ and $\boldsymbol{\theta}_p^{k+1}$, and update u^{k+1} by
$$u^{k+1}(x,t) = \frac{1}{\alpha+\beta}\big(-\hat{p}(x,t;\boldsymbol{\theta}_p^{k+1}) + \lambda^k(x,t) + \beta z^k(x,t)\big).$$

ADMM-PINNs

- **Input:** $\beta > 0$, $z^0, \lambda^0, \boldsymbol{\theta}_y^0, \boldsymbol{\theta}_p^0$.
- For $k \geq 1$
- Update u^{k+1} by the above PINNs.
- Update z^{k+1} by $z^{k+1}(x,t) = \mathbb{P}_{U_{ad}}\left(\mathbb{S}_{\frac{\rho}{\beta}}\left(u^{k+1}(x,t) - \frac{\lambda^k(x,t)}{\beta}\right)\right)$.
- Update $\lambda^{k+1}(x,t) = \lambda^k(x,t) - \beta(u^{k+1}(x,t) - z^{k+1}(x,t))$.
- **Output:** Parameters $(\boldsymbol{\theta}_y^*, \boldsymbol{\theta}_p^*)$ and hence approximate solutions $\hat{y}(x,t;\boldsymbol{\theta}_y^*)$ and $\hat{u}(x,t) = \frac{1}{\alpha+\beta}(-\hat{p}(x,t;\boldsymbol{\theta}_p^*) + \lambda^k(x,t) + \beta z^k(x,t))$.

Numerical Experiments-Problem Setting

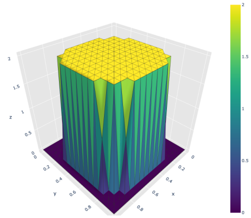
- Set $\Omega = (0,1)^2$, $T = 1, \nu = 1, c_0 = 0, a = -1, b = 2, \bar{y} = 5\sqrt{\rho}t\sin(3\pi x_1)\sin(\pi x_2), \bar{p} = 5\sqrt{\rho}(t-1)\sin(\pi x_1)\sin(\pi x_2)$, and

$$\bar{u} = \begin{cases} \max\{\dfrac{-\bar{p}+\rho}{\alpha}, a\} & \text{in } \{(x,t) \in \Omega \times (0,T) : \bar{p}(x,t) > \rho\}, \\ \min\{\dfrac{-\bar{p}-\rho}{\alpha}, b\} & \text{in } \{(x,t) \in \Omega \times (0,T) : \bar{p}(x,t) < -\rho\}, \\ 0 & \text{otherwise.} \end{cases}$$

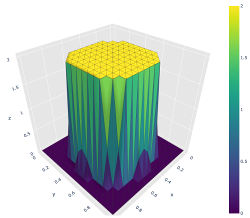
- We further set $f = \frac{\partial \bar{y}}{\partial t} - \Delta \bar{y} - u$ and $y_d = \bar{y} - (-\frac{\partial \bar{p}}{\partial t} - \Delta \bar{p})$.
- Then it can be shown that $\bar{u}$ is the optimal control and $\bar{y}$ is the corresponding optimal state.

Numerical Experiments- Neural Networks and Training

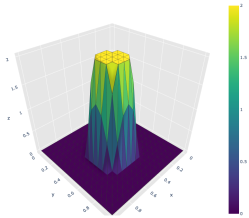
- We approximate y and p with fully-connected feed-forward neural networks containing 3 hidden layers of 32 neurons each. The hyperbolic tangent activation function is used in all the neural networks.
- We uniformly sample $|\mathcal{T}_i| = 4096$ residual points in the spatial-temporal domain $\Omega \times (0, T)$, and $|\mathcal{T}_{b_1}| = 1024$ points in $\partial\Omega \times (0, T)$ and $|\mathcal{T}_{b_2}| = 256$ points in Ω for the boundary and initial conditions.
- The weights are set as $w_y = w_p = 1$, $w_i = 1$ and $w_{b1} = w_{b2} = 5$.
- To train the neural networks, we first use the Adam optimizer with learning rate $\eta = 10^{-3}$ for 10000 iterations, and then switch to the L-BFGS for 10 iterations.
- We execute 10 ADMM iterations with $\alpha = 0.1, \rho = 0.8, \beta = 0.1$, $z^0 = 0$ and $\lambda^0 = 0$.



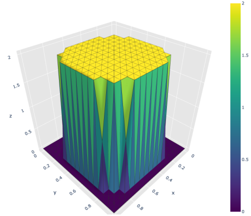
(a) Exact control at $t = 0.25$



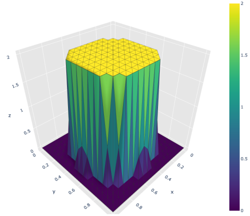
(b) Exact control at $t = 0.5$



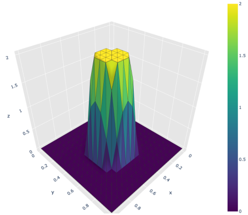
(c) Exact control at $t = 0.75$



(d) Computed control at $t = 0.25$



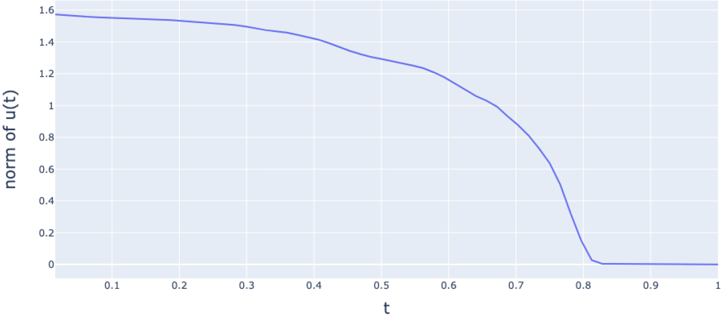
(e) Computed control at $t = 0.5$



(f) Computed control at $t = 0.75$

Numerical Results - Temporal Sparsity

- It is easy to see $\bar{u} = 0$ in $\{(x,t) \in \Omega \times (0,T) : \bar{p}(x,t) < \rho\}$ and we can show that when $t > t^* = 0.8211$, $u(x,t) = 0$ a.e. in Ω.



- The relative error $\frac{\|u^k(x,t) - \bar{u}(x,t)\|_{L^2(Q)}}{\|\bar{u}(x,t)\|_{L^2(Q)}} = 1.45 \times 10^{-2}$.

Comments on ADMM-PINNs

- The ADMM-PINNs approach substantially enlarges the applicable range of PINNs to nonsmooth PDE-constrained optimization problems.
- No need to solve PDEs repeatedly.
- Mesh-free, easy to implement, and scalable to different PDE-constrained optimization problems.[3]

[3] Y. S, Y. Yuan, and H. Yue, "The ADMM-PINNs algorithmic framework for nonsmooth PDE-constrained optimization: a deep learning approach", arXiv preprint arXiv:2302.08309,2023.

The Hard-Constraint PINNs for Elliptic Interface Optimal Control Problems

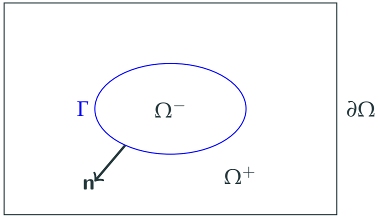
Elliptic Interface Optimal Control-Revisit

- An elliptic interface optimal control problem:

$$\min_{y\in L^2(\Omega),u\in L^2(\Omega)} J(y,u) := \frac{1}{2}\|y-y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)},$$

subject to

$$\begin{cases} -\nabla\cdot(\beta\nabla y) = u+f & \text{in } \Omega\backslash\Gamma, \\ [y]_\Gamma = g_0,\ [\beta\partial_{\boldsymbol{n}} y]_\Gamma = g_1 & \text{on } \Gamma, \\ y = h_0 & \text{on } \partial\Omega, \end{cases}$$



First-Order Optimality Systems

- Let $(u^*, y^*)^\top$ be the solution to the elliptic interface optimal control problem and p^* be the corresponding adjoint variable, then the following first-order optimality system holds:

$$u^* = -\frac{1}{\alpha} p^*,$$

$$\begin{cases} -\nabla \cdot (\beta \nabla y^*) = u^* + f & \text{in } \Omega \backslash \Gamma, \\ [y^*]_\Gamma = g_0, \ [\beta \partial_{\boldsymbol{n}} y^*]_\Gamma = g_1 & \text{on } \Gamma, \\ y^* = h_0 & \text{on } \partial\Omega, \end{cases}$$

$$\begin{cases} -\nabla \cdot (\beta \nabla p^*) = y^* - y_d & \text{in } \Omega \backslash \Gamma, \\ [p^*]_\Gamma = 0, \ [\beta \partial_n p^*]_\Gamma = 0 & \text{on } \Gamma, \\ p^* = 0 & \text{on } \partial\Omega. \end{cases}$$

Smooth Extension

- First, the function $y : \Omega \to \mathbb{R}$ is only piecewise-smooth, but it can be extended to a $(d+1)$-dimensional function $\tilde{y}(x, z) : \Omega \times \mathbb{R} \to \mathbb{R}$, which is smooth on the domain $\Omega \times \mathbb{R}$ and satisfies

$$y(x) = \begin{cases} \tilde{y}(x, 1), & \text{if } x \in \Omega^+, \\ \tilde{y}(x, -1), & \text{if } x \in \Omega^-, \end{cases}$$

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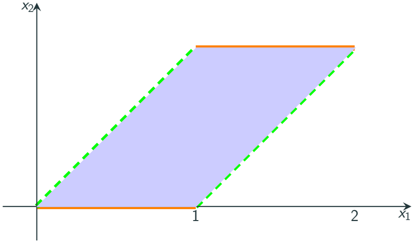

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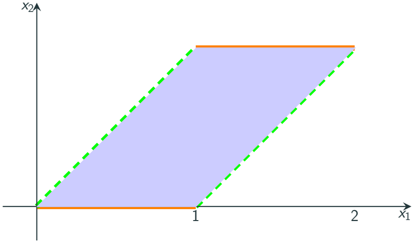

- Similarly, one can extend p to a $(d+1)$-dimensional smooth function $\tilde{p}(x,z)$.

Smooth Extension -Cont'd

- Substituting $\tilde{y}$ and $\tilde{p}$ into the first-order optimality system, we obtain that

$$
\begin{cases}
-\Delta_x \tilde{y}(x,z) = \begin{cases} \dfrac{1}{\beta^+}\left(f(x) + \left(-\dfrac{1}{\alpha}\tilde{p}(x,z)\right)\right) & \text{if } x \in \Omega^+, z = 1 \\ \dfrac{1}{\beta^-}\left(f(x) + \left(-\dfrac{1}{\alpha}\tilde{p}(x,z)\right)\right) & \text{if } x \in \Omega^-, z = -1 \end{cases}, \\
\tilde{y}(x,1) - \tilde{y}(x,-1) = g_0(x), \quad \boldsymbol{n}\cdot(\beta^+\nabla_x \tilde{y}(x,1) - \beta^-\nabla_x \tilde{y}(x,-1)) = g_1(x), \quad \text{if } x \in \Gamma, \\
-\Delta_x \tilde{p}(x,z) = \begin{cases} \dfrac{1}{\beta^+}(\tilde{y}(x,z) - y_d(x)) & \text{if } x \in \Omega^+, z = 1 \\ \dfrac{1}{\beta^-}(\tilde{y}(x,z) - y_d(x)) & \text{if } x \in \Omega^-, z = -1 \end{cases}, \\
\tilde{p}(x,1) - \tilde{p}(x,-1) = 0, \quad \boldsymbol{n}\cdot(\beta^+\nabla_x \tilde{p}(x,1) - \beta^-\nabla_x \tilde{p}(x,-1)) = 0, \quad \text{if } x \in \Gamma, \\
\tilde{y}(x,1) = h_0(x), \quad \tilde{p}(x,1) = 0 \quad \text{if } x \in \partial\Omega.
\end{cases}
$$

Discontinuity Capturing Shallow Neural Networks

- Since $\tilde{y}$ and $\tilde{p}$ are continuous in $\Omega \times \mathbb{R}$, it follows from the universal approximation theorem [Cybenko,1989] that one can approximate them by two shallow neural networks $\hat{y}(x, z; \theta_y)$ and $\hat{p}(x, z; \theta_p)$.

Discontinuity Capturing Shallow Neural Networks

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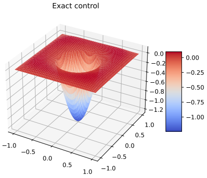
- Such neural networks are referred to as the Discontinuity Capturing Shallow Neural Networks (DCSNN) [Hu, Lin, and Lai, 2022].
- PINNs can be applied!

PINNs

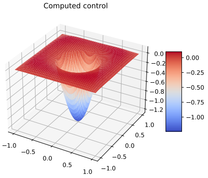
- Sample $\mathcal{T} := \{(x^i, z^i)\}_{i=1}^{M} \subset (\Omega^+ \times \{1\}) \cup (\Omega^- \times \{-1\})$, $\mathcal{T}_B := \{x_B^i\}_{i=1}^{M_B} \subset \partial\Omega$, and $\mathcal{T}_\Gamma := \{x_\Gamma^i\}_{i=1}^{M_\Gamma} \subset \Gamma$.
- Train the neural networks $\hat{y}(x, z; \theta_y)$ and $\hat{p}(x, z; \theta_p)$ by minimizing the loss function:

$$
\begin{aligned}
\mathcal{L}(\theta_y, \theta_p) = & \frac{w_{y,r}}{M} \sum_{i=1}^{M} \left| -\Delta_x \hat{y}(x^i, z^i; \theta_y) - \frac{(-\frac{1}{\alpha}\hat{p}(x^i, z^i; \theta_p)) + f(x^i)}{\beta^\pm} \right|^2 + \frac{w_{y,b}}{M_b} \sum_{i=1}^{M_b} |\hat{y}(x_B^i, 1; \theta_y) - h_0(x_B^i)|^2 \\
& + \frac{w_{y,\Gamma}}{M_\Gamma} \sum_{i=1}^{M_\Gamma} \left| \hat{y}(x_\Gamma^i, 1; \theta_y) - \hat{y}(x_\Gamma^i, -1; \theta_y) - g_0(x_\Gamma^i) \right|^2 \\
& + \frac{w_{y,\Gamma_n}}{M_\Gamma} \sum_{i=1}^{M_\Gamma} \left| \boldsymbol{n} \cdot (\beta^+ \nabla_x \hat{y}(x_i^\Gamma, 1; \theta_y) - \beta^- \nabla_x \hat{y}(x_i^\Gamma, -1; \theta_y)) - g_1(x_\Gamma^i) \right|^2 \\
& + \frac{w_{p,r}}{M} \sum_{i=1}^{M} \left| -\Delta_x \hat{p}(x_i, z_i; \theta_p) - \frac{\hat{y}(x_i, z_i; \theta_y) - y_d(x_i)}{\beta^\pm} \right|^2 + \frac{w_{p,b}}{M_b} \sum_{i=1}^{M_b} |\hat{p}(x_i^b, 1; \theta_p)|^2 \\
& + \frac{w_{p,\Gamma}}{M_\Gamma} \sum_{i=1}^{M_\Gamma} \left| \hat{p}(x_\Gamma^i, 1; \theta_p) - \hat{p}(x_\Gamma^i, -1; \theta_p) \right|^2 + \frac{w_{p,\Gamma_n}}{M_\Gamma} \sum_{i=1}^{M_\Gamma} \left| \boldsymbol{n} \cdot (\beta^+ \nabla_x \hat{p}(x_i^\Gamma, 1; \theta_p) - \beta^- \nabla_x \hat{p}(x_i^\Gamma, -1; \theta_p)) \right|^2
\end{aligned}
$$

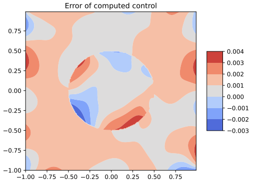
Numerical Results



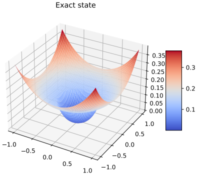
(g) Exact control u.



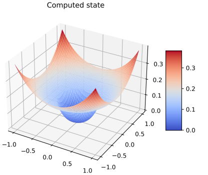
(h) Computed control u.



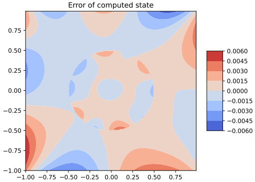
(i) Error of control u.



(j) Exact state y.



(k) Computed state y.



(l) Error of state y.

Hard Constraints- Strategies

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  - Modify the output of the neural network to impose the boundary condition.
  - Construct an auxiliary function for the interface as an additional feature input of the neural network to impose the interface condition.

Hard Constraints - Neural Network Architectures

- Recall that $y = h_0$ on $\partial\Omega$, and $[y]_\Gamma = g_0$.

Hard Constraints - Neural Network Architectures

- Recall that $y = h_0$ on $\partial\Omega$, and $[y]_\Gamma = g_0$.
- We approximate y by

$$\hat{y}(x;\theta_y) = g(x) + h(x)\mathcal{N}_y(x,\phi(x);\theta_y).$$

  - The function $g : \overline{\Omega} \to \mathbb{R}$ satisfies

$$g|_{\partial\Omega} = h_0, \quad [g]_\Gamma = g_0, \quad g|_{\Omega^+} \in C^2(\overline{\Omega^+}), \quad g|_{\Omega^-} \in C^2(\overline{\Omega^-}).$$

  - The function $h : \overline{\Omega} \to \mathbb{R}$ satisfies

$$h \in C^2(\overline{\Omega}), \quad h(x) = 0 \text{ if and only if } x \in \partial\Omega.$$

  - $\phi : \overline{\Omega} \to \mathbb{R}$ is an auxiliary function for the interface Γ and satisfies

$$\phi \in C(\overline{\Omega}), \quad \phi|_{\Omega^+} \in C^2(\overline{\Omega^+}), \quad \phi|_{\Omega^-} \in C^2(\overline{\Omega^-}), [\phi]_\Gamma = 0, \quad [\beta\partial_n\phi]_\Gamma \neq 0 \text{ a.e. on } \Gamma$$

  - $\mathcal{N}_y(x,\phi(x);\theta_y)$ is a neural network with smooth activation functions.

Hard Constraints - Verification

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- $[\hat{y}]_\Gamma(x) = [g]_\Gamma(x) + [h(\cdot)\mathcal{N}_y(\cdot, \phi(\cdot))]_\Gamma(x) = g_0(x), \ \forall x \in \Gamma$ – The interface condition is satisfied.

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- $\hat{y}|_{\partial\Omega}(x) = g|_{\partial\Omega}(x) + h|_{\partial\Omega}(x)\left(\mathcal{N}_y(\cdot, \phi(\cdot))|_{\partial\Omega}\right)(x) = h_0(x), \ \forall x \in \partial\Omega$. – The boundary condition is satisfied.

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- Furthermore, we have

$$
\begin{aligned}
[\beta\partial_{\boldsymbol{n}}\hat{y}]_\Gamma(x) &= [\beta\partial_n g]_\Gamma(x) + [\beta\partial_n\mathcal{N}_y(\cdot,\phi(\cdot))]_\Gamma(x) \\
&= [\beta\partial_{\boldsymbol{n}} g]_\Gamma(x) + (\beta^+ - \beta^-)\left(\mathcal{N}_y(x,\phi(x))(\boldsymbol{n}\cdot\nabla h(x)) + h(x)(\boldsymbol{n}\cdot\nabla_x\mathcal{N}(x,\phi(x)))\right) \\
&\quad + \frac{\partial\mathcal{N}_y}{\partial\phi}\left(h(x)[\beta\partial_{\boldsymbol{n}}\phi]_\Gamma(x)\right), \quad \forall x \in \Gamma,
\end{aligned}
$$

which implies that the interface-gradient condition $[\beta\partial_{\boldsymbol{n}} y]_\Gamma = g_1$ cannot be exactly satisfied by $\hat{y}(x;\theta_y)$ and should be penalized in the loss function of PINNs.

Choices of g and h

- If the functions g_0 and h_0, the interface Γ, and the boundary $\partial\Omega$ admit analytic forms, it is usually easy to construct g and h with analytic expressions.
- For instance, if $\Omega = (0,1) \times (0,1)$, then we can choose $h = x_1(1 - x_1)x_2(1 - x_2)$.
- More discussions can be found in e.g., [Lagari, Tsoukalas, Safarkhani, and Lagaris, 2020; Lagaris, Likas, and Fotiadis, 1998; Lu, Pestourie, Yao, Wang, Verdugo, and, Johnson, 2021].

Choice of ϕ

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- If Γ is the zero level set of a function $\psi(x) \in C^2(\Omega)$, then we can define $\phi(x)$ as follows:

$$\phi(x) = \begin{cases} \psi(x), & \text{if } x \in \Omega^-, \\ 0, & \text{if } x \in \Omega^+ \cup \Gamma \cup \partial\Omega, \end{cases}$$

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- (Circle-shaped Interface) Consider a domain $\Omega \subset \mathbb{R}^d$ and the interface $\Gamma \subset \Omega$ is given by the circle $\Gamma = \{x \in \mathbb{R}^{d-1} : \|x\|_2 = r_0\}$, with $r_0 > 0$. The domain Ω is divided into two parts $\Omega^- = \{x \in \mathbb{R}^{d-1} : \|x\|_2 < r_0\}$ and $\Omega^+ = \{x \in \Omega : \|x\|_2 > r_0\}$. In this case, Γ is the zero level set of $\psi(x) = r_0^2 - \|x\|_2^2$, and the auxiliary function ϕ can be defined as

$$\phi(x) = \begin{cases} \psi(x), & \text{if } x \in \Omega^- \\ 0, & \text{if } x \in \Omega^+ \cup \Gamma \cup \partial\Omega. \end{cases}$$

Choice of ϕ - Cont'd

Choice of ϕ - Cont'd

- The above idea can be easily extended to the case where Γ is a finite union of the zero level sets of some functions $\psi_1, \ldots, \psi_n \in C^2(\overline{\Omega^-})(n \geq 1)$.

Choice of ϕ - Cont'd

- The above idea can be easily extended to the case where Γ is a finite union of the zero level sets of some functions $\psi_1, \ldots, \psi_n \in C^2(\overline{\Omega^-})(n \geq 1)$.
- (Box-shaped Interface) Consider a domain $\Omega \subset \mathbb{R}^d$ containing the box $B := [a_1, b_1] \times \cdots \times [a_d, b_d] \in \mathbb{R}^d$. Let the interface $\Gamma = \partial B$, which divides Ω into $\Omega^- = (a_1, b_1) \times \cdots \times (a_d, b_d)$ and $\Omega^+ = \Omega \backslash B$. In this case, we define

$$\phi(x) = \begin{cases} \prod_{i=1}^d (x_i - a_i)(b_i - x_i), & \text{if } x \in \Omega^-, \\ 0, & \text{if } x \in \Omega^+ \cup \Gamma \cup \partial\Omega. \end{cases}$$

- Otherwise, we shall show that, if Ω^+, Ω^-, and Γ satisfy the following assumptions, then we can construct an auxiliary function $\phi(x)$ analytically.

Assumptions

- The sub-domain Ω^- is the intersection of the interior of finitely many oriented, smooth, and embedded manifolds $M_1, M_2, \ldots, M_n$, where $M_i \cap M_j$ is of measure zero whenever $i \neq j$ and $i, j \in \{1, \ldots, n\}$.
- There exists an open neighborhood $U \subset \mathbb{R}^d$ of Γ, such that for each M_i $(i \in \{1, \ldots, n\})$, there exists smooth functions $\psi_i : U \to \mathbb{R}$ satisfying $\psi_i \in C^2(\overline{U})$ and

$$\psi_i(x) = 0 \text{ if } x \in \Gamma, \quad \psi_i(x) > 0 \text{ if } x \in U \cap \Omega^-, \quad \partial_{\boldsymbol{n}} \psi_i \neq 0 \text{ on } M_i \cap \Gamma.$$

- There exists constants $c_i > 0$ such that $\psi_i(x) > c_i$ for all $x \in \partial U \cap \overline{\Omega^-}$ and for all $i \in \{1, \ldots, n\}$.

Choice of ϕ - Cont'd

Theorem

Suppose the above assumptions hold and we define $\psi : U \to \mathbb{R}$ as $\psi(x) = \prod_{i=1}^{n} \psi_i(x)$. For any constant c such that $0 < c < \prod_{i=1}^{n} c_i$, let

$$L_c := \{x \in U : \psi(x) \geq c\}.$$

Then the function $\phi : \bar{\Omega} \to \mathbb{R}$ given by

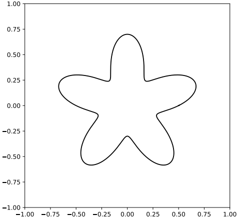
$$\phi(x) = \begin{cases} c^3, & \text{if } x \in (\overline{\Omega^-} \backslash U) \cup (\overline{\Omega^-} \cap L_c), \\ c^3 - (c - \psi(x))^3, & \text{if } x \in (U \cap \overline{\Omega^-}) \backslash L_c, \\ 0, & \text{if } x \in \overline{\Omega^+} \end{cases}$$

is well-defined and satisfies

$$\phi \in C(\overline{\Omega}), \quad \phi|_{\Omega^+} \in C^2(\overline{\Omega^+}), \quad \phi|_{\Omega^-} \in C^2(\overline{\Omega^-}), [\phi]_\Gamma = 0, \quad [\beta \partial_n \phi]_\Gamma \neq 0 \text{ a.e. on } \Gamma.$$

- Let $\Omega \subset \mathbb{R}^2$ be a bounded domain and the star-shaped interface $\Gamma \subset \mathbb{R}$ be defined by the zero level set of the following function in polar coordinates $\psi(r,\theta) = r - a - b\sin(5\theta)$ with constants $b < a$. The domain Ω is divided into $\Omega^- = \{(r,\theta) \in \mathbb{R}^2 : r < a + b\sin(5\theta)\}$ and $\Omega^+ = \{(r,\theta) \in \Omega : r > a + b\sin(5\theta)\}$.
- Note that $\psi(r,\theta)$ is not differentiable on Ω, since the polar angle is not differentiable at the origin. In this case, we define

$$\phi(r,\theta) = \begin{cases} \left(\frac{a-b}{2}\right)^3, & \text{if } a + b\sin(5\theta) - r \geq \frac{a-b}{2}, \\ \left(\frac{a-b}{2}\right)^3 - \left(\frac{a-b}{2} + \psi(r,\theta)\right)^3, & \text{if } 0 < a + b\sin(5\theta) - r < \frac{a-b}{2}, \\ 0, & \text{otherwise.} \end{cases}$$



Remarks on the Choices of Auxiliary Functions

- If the functions g, h, and ϕ are difficult to construct analytically, we can construct them by training some neural networks.

Remarks on the Choices of Auxiliary Functions

- If the functions g, h, and ϕ are difficult to construct analytically, we can construct them by training some neural networks.
- For instance, we can train a DCSNN $\hat{g}(x, z; \theta_g)$ and a neural network $\hat{h}(x; \theta_h)$ with smooth activation functions by minimizing the following loss functions:

$$\frac{w_{1g}}{M_b} \sum_{i=1}^{M_b} |\hat{g}(x_B^i, 1; \theta_y) - h_0(x_B^i)|^2 + \frac{w_{2g}}{M_\Gamma} \sum_{i=1}^{M_\Gamma} \left|\hat{g}(x_\Gamma^i, 1; \theta_g) - \hat{g}(x_\Gamma^i, -1; \theta_g) - g_0(x_\Gamma^i)\right|^2,$$

and

$$\frac{w_{1h}}{M_b} \sum_{i=1}^{M_b} |\hat{h}(x_B^i; \theta_h)|^2 + \frac{w_{2h}}{M} \sum_{i=1}^{M} |\hat{h}(x^i; \theta_h) - \bar{h}(x^i)|^2,$$

  - w_{1g}, w_{2g}, w_{1h}, and $w_{2h} > 0$ are the weights.
  - $\{x^i\}_{i=1}^M \subset \Omega$, $\{x_B^i\}_{i=1}^{M_B} \subset \partial\Omega$, and $\{x_\Gamma^i\}_{i=1}^{M_\Gamma} \subset \Gamma$ are the training points.
  - $\bar{h}(x) \in C^2(\Omega)$ is a known function satisfying $\bar{h}(x) \neq 0$ in Ω, e.g. $\bar{h}(x) = \min_{\hat{x} \in \partial\Omega} \{\|x - \hat{x}\|_2^4\}$.

The Hard-Constraint PINNs

- We approximate y by the neural network $\hat{y}(x;\theta_y) = g(x) + h(x)\mathcal{N}_y(x, \phi(x); \theta_y)$ defined above.

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- Since the boundary and interface conditions for p are homogeneous, we approximate it by

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The Hard-Constraint PINNs

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$$\hat{p}(x;\theta_p) = h(x)\mathcal{N}_p(x,\phi(x);\theta_p).$$

- The neural networks $\hat{y}(x;\theta_y)$ and $\hat{p}(x;\theta_p)$ are trained by minimizing

$$\begin{aligned}\mathcal{L}_{HC}(\theta_y,\theta_p) =& \frac{w_{y,r}}{M}\sum_{i=1}^{M}\left|-\Delta_x\hat{y}(x^i;\theta_y) - \frac{(-\frac{1}{\alpha}\hat{p}(x^i;\theta_p)) + f(x^i)}{\beta^{\pm}}\right|^2 + \frac{w_{y,\Gamma_n}}{M_\Gamma}\sum_{i=1}^{M_\Gamma}\left|[\beta\partial_{\boldsymbol{n}}\hat{y}]_\Gamma(x_\Gamma^i;\theta_y) - g_1(x_\Gamma^i)\right|^2 \\ &+ \frac{w_{p,r}}{M}\sum_{i=1}^{M}\left|-\Delta_x\hat{p}(x_i;\theta_p) - \frac{\hat{y}(x_i;\theta_y) - y_d(x_i)}{\beta^{\pm}}\right|^2 + \frac{w_{p,\Gamma_n}}{M_\Gamma}\sum_{i=1}^{M_\Gamma}\left|[\beta\partial_{\boldsymbol{n}}\hat{p}]_\Gamma(x_i^\Gamma;\theta_p)\right|^2.\end{aligned}$$

Numerical Comparisons

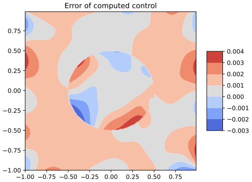
- To test the accuracy, we select 256×256 testing points $\{x^i\}_{i=1}^{M_T} \subset \Omega$ following the Latin hypercube sampling.
- Then compute

$$\varepsilon_{\text{abs}} = \sqrt{\frac{1}{M_T}\sum_{i=1}^{M_T}(\hat{u}(x^i) - u^*(x^i))^2}, \text{ and } \varepsilon_{rel} = \varepsilon_{abs}\sqrt{A(\Omega)}/||u^*||_{L^2(\Omega)}$$

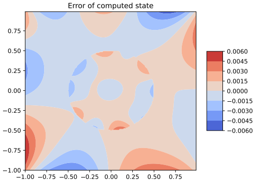
where $A(\Omega)$ is the area of Ω (i.e. the Lebesgue measure of Ω), and $||u^*||_{L^2(\Omega)}$ is computed using the numerical integration function `dblquad` implemented in the SciPy library of Python.
- The soft-constraint PINNs: $\varepsilon_{\text{abs}} = 1.2360 \times 10^{-3}$, $\varepsilon_{\text{rel}} = 4.0461 \times 10^{-3}$
- The hard-constraint PINNs: $\varepsilon_{\text{abs}} = 4.7652 \times 10^{-5}$, $\varepsilon_{\text{rel}} = 1.5599 \times 10^{-4}$
- The hard-constraint PINNs approach improves the accuracy by more than 20x.

Numerical Comparisons

- Numerical errors of the soft-constraint PINNs.

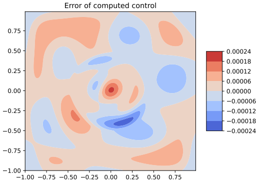


(m) Error of control u.

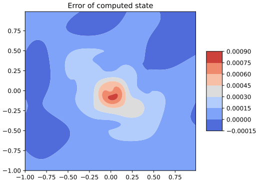


(n) Error of state y.

- Numerical errors of the hard-constraint PINNs.



(o) Error of control u.



(p) Error of state y.

Comments on the Hard-Constraint PINNs

[4] M. Lai, Y. Song, X. Yuan, H. Yue, and T. Zeng. "The hard-constraint physics-informed neural networks for interface optimal control problems". arXiv preprint arXiv:2308.06709.

Comments on the Hard-Constraint PINNs

- The boundary and interface conditions can be satisfied exactly and they are decoupled from the learning of the PDEs.

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Comments on the Hard-Constraint PINNs

- The boundary and interface conditions can be satisfied exactly and they are decoupled from the learning of the PDEs.
- This hard-constraint approach significantly simplifies the training process and enhances the numerical accuracy.
- The resulting algorithm is mesh-free, easy to implement, and scalable to different interface optimal control problems.[4]

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Conclusions and Perspectives

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Conclusions

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- Combine PINNs with classic operator splitting optimization techniques (e.g., ADMM) leads to implementable and efficient algorithms for PDE-constrained optimization problems with nonsmooth objective functional.
- Leveraged by the discontinuity capturing neural networks, PINNs can be applied to solve interface optimal control problem.
- Imposing the boundary and interface conditions as hard constraints can improve the numerical accuracy and simplify the training procedure of PINNs.

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- Develop new computational tools for data-driven/physics-informed modeling, combining machine learning and optimization techniques, motivated by relevant applications in physics engines and digital twins.

Perspectives

- The validated efficiency of the ADMM-PINNs and the hard-constraint PINNs clearly justifies the necessity to investigate the underlying theoretical issues such as convergence analysis and error estimate.
- Develop new computational tools for data-driven/physics-informed modeling, combining machine learning and optimization techniques, motivated by relevant applications in physics engines and digital twins.
- Make a breakthrough on the mathematical foundations of machine learning-based computational methods, through the systematic development of new ideas and methods of control theoretical inspiration.


Danke
Merci
Cảm ơn bạn
Teşekkür ederiz
Grazie
谢谢
Obrigado
謝謝
Gracias
Thank you
شكرا
Terima kasih
धन्यवाद
ధన్యవాదాలు
Спасибо
شكرا
நன்றி
धन्यवाद
ありがとう
ขอบคุณ
감사합니다