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

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Background and Motivation

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- PDE-constrained optimization problems arise.

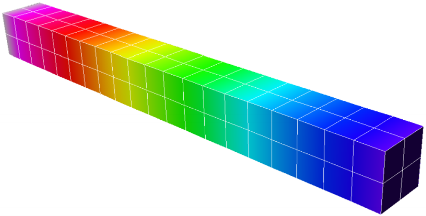

Figure 1: Control the heat distribution of a metal bar

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

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- A parabolic sparse optimal control problem:

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

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 $\alpha > 0$, $\rho > 0$ and the coefficients $\nu > 0$, $c_0 \geq 0$ are 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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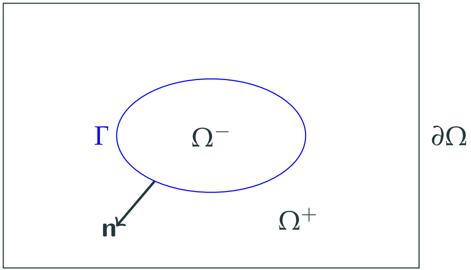

Figure 2: The geometry of an interface problem: an illustration

Nonsmooth PDE-Constrained Optimization-II

- 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 functions $f\in L^2(\Omega), g_0\in H^{\frac{1}{2}}(\Gamma), g_1\in L^2(\Gamma)$, and $h_0\in H^{\frac{1}{2}}(\partial\Omega)$ are given, and β is a nonzero piecewise-constant in $\Omega\backslash\Gamma$ such that $\beta=\beta^-$ in Ω^- and $\beta=\beta^+$ in Ω^+.
- The jump discontinuity across Γ: $[y]_\Gamma(x) := \lim_{\tilde{x}\to x \text{ in } \Omega^+} y(\tilde{x}) - \lim_{\tilde{x}\to x \text{ in } \Omega^-} y(\tilde{x}), \forall x\in\Gamma$.
- 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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3. Specify a loss function by summing the residuals of the PDE and the boundary condition:

$$\mathcal{L}_{PDE}(\boldsymbol{\theta}, \mathcal{T}) = w_i \mathcal{L}_i(\boldsymbol{\theta}, \mathcal{T}_i) + w_b \mathcal{L}_b(\boldsymbol{\theta}, \mathcal{T}_b),$$

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 and w_b 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.

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- More applications and discussions about PINNs can be referred to the review papers:
  - Cuomo, S., Di Cola, V. S., Giampaolo, F., Rozza, G., Raissi, M., and Piccialli, F. *Scientific Machine Learning Through Physics–Informed Neural Networks: Where we are and What's Next.* J Sci Comput 92, 88 (2022).
  - Faroughi, S. A., Pawar, N., Fernandes, C., Das, S., Kalantari, N. K., and Mahjour, S. K. *Physics-Guided, Physics-Informed, and Physics-Encoded Neural Networks in Scientific Computing.* arXiv preprint, arXiv:2211.07377, (2022).
  - Hao, Z., Liu, S., Zhang, Y., Ying, C., Feng, Y., Su, H., and Zhu, J. *Physics-Informed Machine Learning: A Survey on Problems, Methods and Applications*. arXiv preprint arXiv:2211.08064, (2022).
  - Karniadakis, G. E., Kevrekidis, I. G., Lu, L., Perdikaris, P., Wang, S., and Yang, L. *Physics-informed machine learning.* Nature Reviews Physics, 3(6) (2021) 422-440.
  - Lu, L., Meng, X., Mao, Z., and Karniadakis, G.E. *DeepXDE: A deep learning library for solving differential equations.* SIAM Rev. 63 (1) (2021) 208-228.

PINNs for Smooth PDE-Constrained Optimization

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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 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.
- The PDE constraint and the nonsmooth regularization are treated individually.
- The resulting subproblems admit closed-form solution or can be solved directly by some well-developed computational techniques (e.g., PINNs).

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- Let $y(u)$ be the solution of the parabolic state equation corresponding to u. Introduce $z \in L^2(Q)$ satisfying $u = z$, we then have

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

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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:

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

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- The z-subproblem is

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

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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: $\mathbb{S}_\zeta(v)(x) = \operatorname{sgn}(v(x))(|v(x)| - \zeta)_+, \forall\, \zeta > 0.$

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 $u^{k+1}(x,t) = \frac{1}{\alpha+\beta}(-\hat{p}(x,t;\boldsymbol{\theta}_p^{k+1}) + \lambda^k(x,t) + \beta z^k(x,t))$.

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

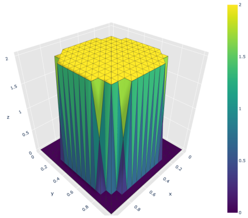
$$\bar{u} = \begin{cases} \max\{\dfrac{-\bar{p}+\rho}{\alpha}, a\} & \text{in } \{(x,t) \in \Omega \times (0,T) : \bar{p}(x,t) > \rho\}, \\ \min\{\dfrac{-\bar{p}-\rho}{\alpha}, b\} & \text{in } \{(x,t) \in \Omega \times (0,T) : \bar{p}(x,t) < -\rho\}, \\ 0 & \text{otherwise.} \end{cases}$$

- 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.

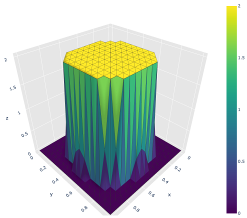
Numerical Experiments- Neural Networks and Training

- 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 $\lambda^0 = 0$.

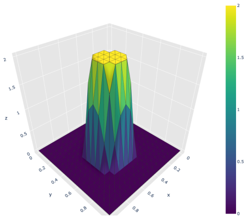
Numerical Results - Spatial Sparsity



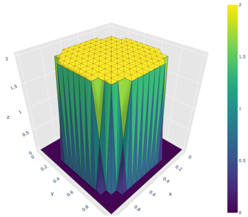
(a) Exact control at $t = 0.25$



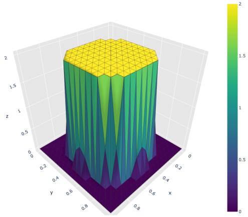
(b) Exact control at $t = 0.5$



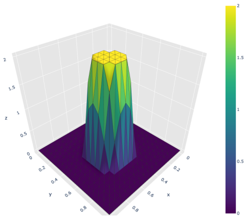
(c) Exact control at $t = 0.75$



(d) Computed control at $t = 0.25$



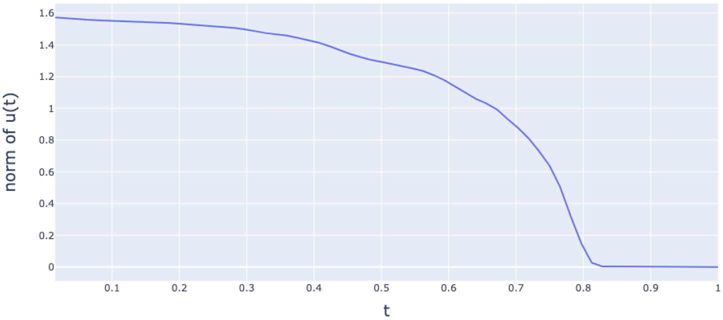
(e) Computed control at $t = 0.5$



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

Extensions of ADMM-PINNs

- More applications of the ADMM-PINNs and numerical results can be found in *Y. Song, 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

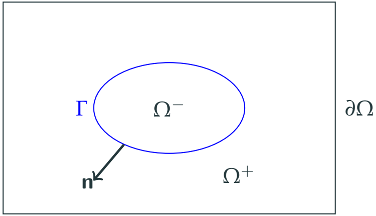
Elliptic Interface Optimal Control-Revisit

- 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:

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

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

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

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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- The additional input $z \in \mathbb{R}$ is the augmented coordinate variable that labels Ω^+ and Ω^-.

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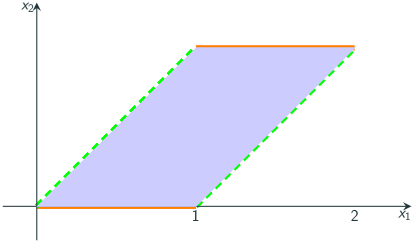

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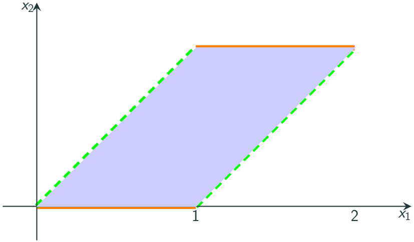

- Similarly, one can extend p to a $(d+1)$-dimensional smooth function $\tilde{p}(x, z)$.

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 $\hat{p}(x, z; \theta_p)$.

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

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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:

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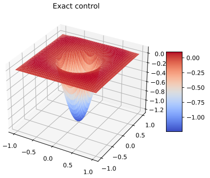
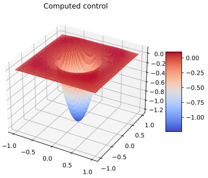
$$

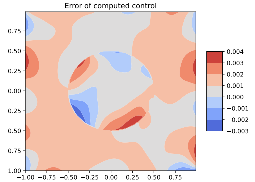
Numerical Results



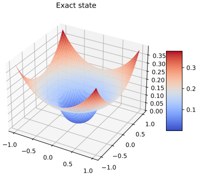
(g) Exact control u.



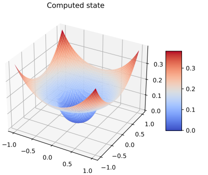
(h) Computed control u.



(i) Error of control u.



(j) Exact state y.



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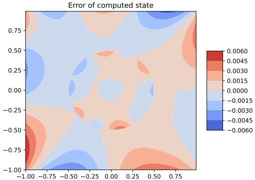

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  - The above numerical results show that the numerical errors mainly accumulate on the boundaries and the interfaces.
- To tackle the above issues, we consider imposing the boundary and interface conditions as hard constraints so that they are satisfied exactly and can be treated separately from the PDE in the training of the neural networks.

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

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- 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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- Furthermore, we have

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

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 Auxiliary Functions

- 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].

Choices of Auxiliary Functions - Cont'd

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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, the auxiliary function ϕ can be constructed as

$$\phi(x) = \begin{cases} r_0^2 - \|x\|_2^2, & \text{if } x \in \Omega^- \\ 0, & \text{if } x \in \Omega^+ \cup \Gamma \cup \partial\Omega. \end{cases}$$

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- (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 $i \in \{1, \ldots, n\}$.

Choices of Auxiliary Functions - 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

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

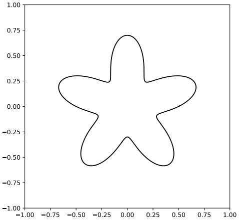
is well-defined and satisfies

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

An Example of ϕ

- 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

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



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.

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- 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

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

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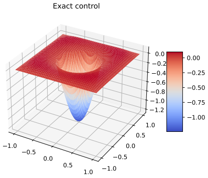
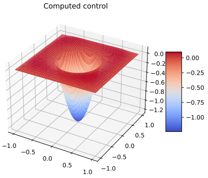
- The neural networks $\hat{y}(x;\theta_y)$ and $\hat{p}(x;\theta_p)$ are trained by minimizing

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

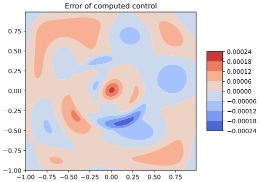
Numerical Results



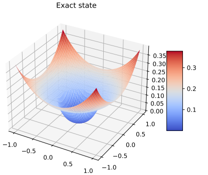
(m) Exact control u.



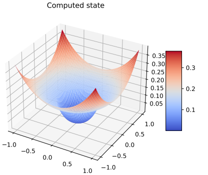
(n) Computed control u.



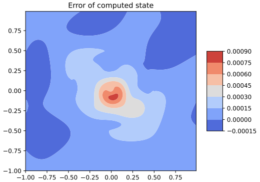
(o) Error of control u.



(p) Exact state y.



(q) Computed state y.



(r) Error of state y.

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

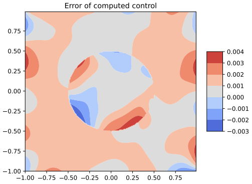
$$\varepsilon_{\text{abs}} = \sqrt{\frac{1}{M_T}\sum_{i=1}^{M_T}(\hat{u}(x^i) - u^*(x^i))^2}, \text{ and } \varepsilon_{rel} = \varepsilon_{abs}\sqrt{A(\Omega)}/||u^*||_{L^2(\Omega)}$$

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.

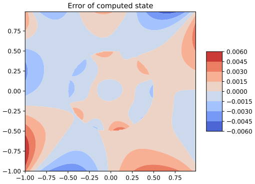
- The soft-constraint PINNs: $\varepsilon_{\text{abs}} = 1.2360 \times 10^{-3}$, $\varepsilon_{\text{rel}} = 4.0461 \times 10^{-3}$
- The hard-constraint PINNs: $\varepsilon_{\text{abs}} = 4.7652 \times 10^{-5}$, $\varepsilon_{\text{rel}} = 1.5599 \times 10^{-4}$
- The hard-constraint PINNs approach improves the accuracy by more than 20x.

Numerical Comparisons

- Numerical errors of the soft-constraint PINNs.

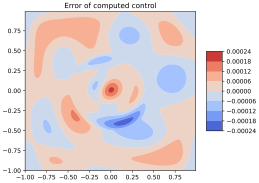


(s) Error of control u.

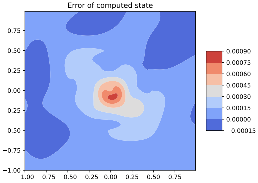


(t) Error of state y.

- Numerical errors of the hard-constraint PINNs.



(u) Error of control u.



(v) Error of state y.

More Results

- More numerical results on the hard-constraint PINNs for solving other interface optimal control problems can be found in
  M. Lai, Y. Song, X. Yuan, H. Yue, and T. Zeng. "The hard-constraint physics-informed neural networks for interface optimal control problems". to appear

Conclusions and Perspectives

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- The validated efficiency of the ADMM-PINNs and the hard-constraint PINNs clearly justifies the necessity to investigate the underlying theoretical issues such as the convergence analysis and the error estimate.


Danke
Merci
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Grazie
谢谢
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謝謝
Thank you
شكرا
Gracias
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धन्यवाद
ధన్యవాదాలు
Спасибо
شكرا
நன்றி
धन्यवाद
ありがとう
ขอบคุณ
감사합니다