Deep Neural ODE Operator Networks for PDEs

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Outline

Outline

PDEs and Traditional Numerical solvers

- We consider a generic class of PDEs modeled by

$$\begin{cases} \partial_t u(t,x) + \mathcal{L}[a](u)(t,x) = f(t,x) & \forall (t,x) \in [0,T] \times \Omega, \\ u(0,x) = u_0(x) & \forall x \in \Omega, \\ \mathcal{B}u(t,x) = u_b(t,x) & \forall (t,x) \in [0,T] \times \partial\Omega. \end{cases}$$

  A numerical solver of the PDE tries to find the numerical approximation of

$$(t,x) \to u \approx u_\theta.$$

- **Traditional Numerical Methods:**
  - Finite Element Method (FEM),
  - Finite Difference Method (FDM),
  - Finite Volumn Method (FVM).
- **Challenges of Traditional Methods:**
  - PDEs in high-dimensional spaces and complex domains.
  - Problems requiring repeated but expensive simulations, e.g., inverse problems and optimal control of PDEs.

Scientific Machine Learning for PDEs - function learning

Solution learning methods: using NNs to approximate the solution function of a PDE

- Deep Ritz method [E and Yu, 2017]
- Deep Galerkin method [Sirignano and Spiliopoulos, 2017]
- Physics-informed neural networks (PINNs) [Raissi, Perdikaris, and Karniadakis, 2017]
- Weak adversarial networks [Zang, Bao, Ye, and Zhou, 2019]
- Random feature methods [Chen, Chi, E, and Yang, 2022]
- ... ...

Typical applications:

- High-dimensional PDEs.
- Complex geometries.
- ... ...

Operator Learning

We consider a class of non-stationary PDEs modeled by

$$\begin{cases} \partial_t u(t,x) + \mathcal{L}[a](u)(t,x) = f(t,x) & \forall (t,x) \in [0,T] \times \Omega, \\ u(0,x) = u_0(x) & \forall x \in \Omega, \\ \mathcal{B}u(t,x) = u_b(t,x) & \forall (t,x) \in [0,T] \times \partial\Omega. \end{cases}$$

- **Parameters:** $v \subset \{f, a, u_0, u_b\}$.
- **Goal of operator learning:**

$$\Psi_\theta \approx \Psi^\dagger : v \mapsto u,$$

where $\Psi^\dagger$ is the solution operator , which maps v to the solution u, by a neural-network–based functional Ψ_θ with trainable parameters θ.

Scientific Machine Learning for PDEs - operator learning

Operator learning methods: using NNs to approximate the solution operator of a PDE

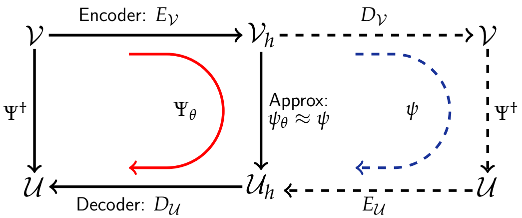
- Deep Operator Networks (DeepONets) [Lu, Jin, Pang, Zhang, and Karniadakis, 2019],
- Physics-Informed DeepONets [Wang, Wang, and Perdikaris, 2021]
- Fourier Neural Operator, Graph Neural Operator, [Li, Kovachki, Azizzadenesheli, Liu, Bhattacharya, Stuart, and Anandkumar,2021]
- The Random Feature Approach [Nelsen and Stuart, 2021]
- In-Context Operator Networks [Yang, Liu, Meng, and Osher, 2024]
- ... ...

Typical applications:

- PDEs discovery: model and predict unknown physics through data.
- Acceleration: speed-up computationally expensive simulations.
- ... ...

Encoder-decoder-net architectures

- Learning an infinite-dimensional operator $\Psi^\dagger : \mathcal{V} \to \mathcal{U}$.



- An encoder-decoder pair $(E_\mathcal{V}, D_\mathcal{V})$ on $\mathcal{V}$, i.e., $E_\mathcal{V} : \mathcal{V} \to \mathbb{R}^{d_\mathcal{V}}$, $D_\mathcal{V} : \mathbb{R}^{d_\mathcal{V}} \to \mathcal{V}$,
- An encoder-decoder pair $(E_\mathcal{U}, D_\mathcal{U})$ on $\mathcal{U}$, i.e., $E_\mathcal{U} : \mathcal{U} \to \mathbb{R}^{d_\mathcal{U}}$, $D_\mathcal{U} : \mathbb{R}^{d_\mathcal{U}} \to \mathcal{U}$.
- These encoder/decoder pairs imply a finite-dimensional function

$$\psi : \mathcal{V}_h \to \mathcal{U}_h, \quad \psi(\zeta) = E_\mathcal{U} \circ \Psi^\dagger \circ D_\mathcal{V}(\zeta), \quad \forall \zeta \in \mathcal{V}_h$$

and then $D_\mathcal{U} \circ \psi \circ E_\mathcal{V} \approx \Psi^\dagger$.

- Using a neural network $\psi_\theta : \mathcal{V}_h \to \mathcal{U}_h$ to approximate ψ, we obtain an encoder-decoder network $\Psi_\theta : \mathcal{V} \to \mathcal{U}$:

$$\Psi_\theta := D_\mathcal{U} \circ \psi_\theta \circ E_\mathcal{V} \approx \Psi^\dagger.$$

Outline

A concrete example: Heat equation

We consider the 1D heat equation

$$\begin{cases} \partial_t u(t,x) - \Delta u(t,x) = 0, \quad \forall (t,x) \in [0,1] \times [0,1], \\ u(t,0) = u(t,1) = 0, \quad \forall t \in [0,1], \\ u(0,x) = u_0(x), \quad \forall x \in [0,1]. \end{cases}$$

The obective is to use a neural-network–based functional Ψ_θ to learn the mapping:

$$\Psi_\theta \approx \Psi^\dagger : u_0 \mapsto u.$$

Learn from numerical solutions with different initial conditions. (need discretization)

Step 1: Encoding (Discretization and preparing training dataset)

We discretize space and time into uniform mesh:

- Space: $[0,1] \mapsto N_x$ points: $(x_1, x_2, \ldots, x_{N_x})$
- Time: $[0,1] \mapsto N_T$ points: $(t_1, t_2, \ldots, t_{N_T})$

Let N_{u_0} denote the number of samples of u_0, then the training dataset is:

$$\{U_{0,h}^k, U_h^k\}, \quad k = 1, 2, \ldots, N_{u_0}$$

where $U_{0,h} = \big(u_0(x_i)\big)_{i=1}^{N_x} \in \mathbb{R}^{N_x}$, $U_h^k = \big(u(t_j, x_i)\big)_{i=1,j=1}^{N_x,N_T} \in \mathbb{R}^{N_x \times N_T}$. All the training data is computed by the Finite Difference Method (FDM).

Step 2: NODE surrogate (Approximation and training)

Suppose that U_h^k can be seen as values at different times of the solutions of an ODE with initial data $U_{0,h}^k$. We use U_θ to approximate U_h and we present this ODE by the approximation of the following NODE:

$$\begin{cases} \frac{d}{dt} U_\theta = \sum_{p=1}^{P} w_p \circ \sigma(A_p^1 U_\theta + A_p^2 t + B_p), \\ U_\theta(0,x) = U_{0,h} \in \mathbb{R}^n. \end{cases}$$

Then the loss function to train the NODE is:

$$L(\theta) = \frac{1}{N_v N_x N_T} \sum_{k=1}^{N_v} \sum_{i=1}^{N_x} \sum_{j=1}^{N_T} \left| \left(U_\theta^k(t_j)\right)_i - U_h^k(x_i, t_j) \right|^2 + \mathcal{R}(\theta).$$

Here, $\mathcal{R}(\theta)$ is a general regularization term.

Step 3: Decoding (Reconstructe PDE solution)

After the latent dynamics are learned, the PDE solution u is reconstructed from the NODE outputs u_θ

$$u(t,x) \approx u_\theta(t,x) \; = \; \sum_{i=1}^{N_x} \big(U_\theta(t)\big)_i \, \alpha_i(x), \quad \forall (t,x) \in [0,1] \times [0,1],$$

where α_i is the P_1-FEM basis centered at x_i.

General framework for $v \mapsto u$

For a class of non-stationary PDEs modeled by

$$\begin{cases} \partial_t u(t,x) + \mathcal{L}[a](u)(t,x) = f(t,x) & \forall (t,x) \in [0,T] \times \Omega, \\ u(0,x) = u_0(x) & \forall x \in \Omega, \\ \mathcal{B}u(t,x) = u_b(t,x) & \forall (t,x) \in [0,T] \times \partial\Omega. \end{cases}$$

The parameters of the PDE is defined by $v \subset \{f, a, u_0, u_b\}$. The architecture of the NODE-ONet:

$$\textbf{Architecture} \begin{cases} \text{Encoding:} \quad E_{\mathcal{V}}(v) := \{v_\ell(t)\}_{\ell=1}^{d_{\mathcal{V}}} \in \mathbb{R}^{d_{\mathcal{V}}} \text{ for any } t \in [0,T]; \\ \text{Physics-encoded NODE surrogate:} \quad \begin{cases} \dot{\boldsymbol{\psi}}(t) = \mathcal{N}_{\theta_\psi}(\boldsymbol{\psi}(t), \mathcal{P}_v \boldsymbol{v}(t), t), \\ \boldsymbol{\psi}(0) = \mathcal{P}_u \boldsymbol{u}_0 \in \mathbb{R}^{d_{\mathcal{U}}}, \end{cases} \\ \text{Decoding:} \quad \Psi_{\text{NODE-ONet}}(v;\theta)(t,x) = D_{\mathcal{U}}(t,\alpha) = \sum_{j=1}^{d_{\mathcal{U}}} \alpha_j(x)\psi_j(t), \end{cases}$$

with $\{\alpha_j\}_{j=1}^{d_{\mathcal{U}}}$ a set of spatial basis functions.

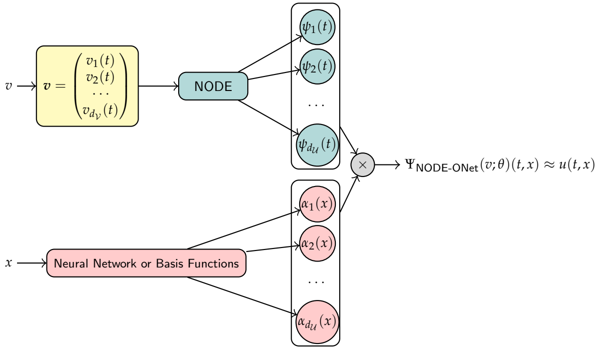
General framework for $v \mapsto u$

The training setting is summarized as follows:

Training:

$$\begin{cases} \text{Dataset: } \{v_i, x_j, \Psi^\dagger(v_i)(t_k, x_j)\}_{1\le i\le N_v, 1\le k\le N_t, 1\le j\le N_x} \\ \text{Loss function: } \mathcal{L}(\theta) = \frac{1}{N_v N_x N_t}\sum_{i=1}^{N_v}\sum_{j=1}^{N_x}\sum_{k=1}^{N_t} \|\Psi_{\text{NODE-ONet}}(v_i)(t_k, x_j) - \Psi^\dagger(v_i)(t_k, x_j)\|_2^2. \end{cases}$$

The generic architure of NODE-ONet:



Outline

1D diffusion-reaction - Setup

We consider the following diffusion-reaction equation

$$\begin{cases} \partial_t u(t,x) - \nabla \cdot (D(t,x)\nabla u(t,x)) + R(t,x)u^2(t,x) = f(t,x) & \forall (t,x) \in [0,T] \times \Omega, \\ u(0,x) = u_0(x) & \forall x \in \Omega, \\ u(t,x) = u_b(t,x) & \forall (t,x) \in [0,T] \times \partial\Omega, \end{cases}$$

In the following experiments, we validate the efficiency of NODE-ONets to approximate the following operators:

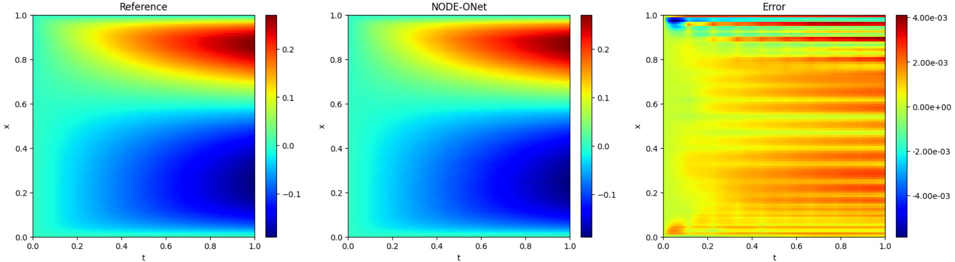
- Source-to-solution operator: $f \mapsto u$. (Comparison with DeepONet)
- Diffusion-to-solution operator: $D \mapsto u$.
- Solution operator with multi-inputs: $\{D, f \mapsto u\}$. (Comparison with MIONet)
- Prediction beyond the training time. (Comparison with DeepONet and MIONet)

1D diffusion-reaction - Source-to-solution operator

- D=0.01.
- Physics-encoded NODE:

$$\begin{cases} \dot{\psi}(t) = \sum_{i=1}^{P} W_i \odot \sigma(A_i \odot \psi + \boldsymbol{a}_i^1 t + B_i) + \mathcal{P}_f \boldsymbol{f}, \\ \psi(0) = \mathbf{0} \in \mathbb{R}^{d_{\mathcal{U}}}. \end{cases}$$

Figure: Test results of the deep NODE operator network for the learned source-to-solution operator $\Psi_f^* : f(x) \to u(x,t)$ with one random $f(x)$.



1D diffusion-reaction - Source-to-solution operator - Comparison

Table: Comparisons of the NODE-ONet with the unstacked DeepONet for learning the source-to-solution operator $\Psi_f^\dagger : f(x) \mapsto u(t,x)$.

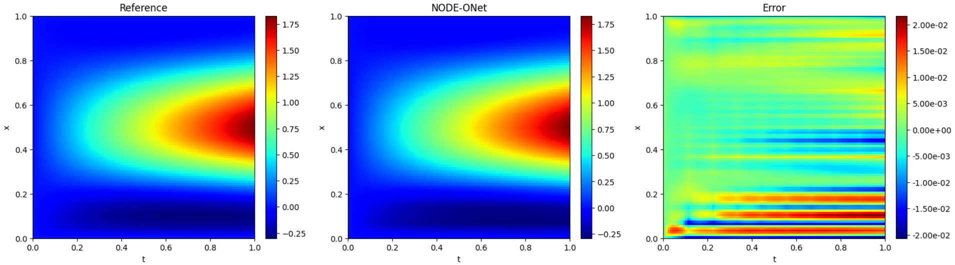
	Training epochs	Training resolutions	#Trainable parameters	#Training input f	Test resolutions	#Test input f	Absolute error	Relative error
NODE-ONet	ADAM 5×10^5	$N_x = 10$ $N_t = 5$ $d_\mathcal{V} = 20$	27,550	100	$N_x = 100$ $N_t = 100$	10,000	4.248×10^{-3}	7.370×10^{-3}
NODE-ONet	ADAM 5×10^5	$N_x = 100$ $N_t = 10$ $d_\mathcal{V} = 20$	27,550	500	$N_x = 100$ $N_t = 100$	10,000	1.368×10^{-3}	2.675×10^{-3}
DeepONet	ADAM 5×10^5	$N_x = 100$ $N_t = 10$ $K = 50$ $d_\mathcal{V} = 100$	40,600	100	$N_x = 100$ $N_t = 100$ $K = 100$	10,000	6.352×10^{-3}	1.230×10^{-2}
DeepONet	ADAM 5×10^5	$N_x = 100$ $N_t = 100$ $K = 1{,}000$ $d_\mathcal{V} = 100$	40,600	500	$N_x = 100$ $N_t = 100$ $K = 1{,}000$	10,000	1.313×10^{-3}	2.582×10^{-3}

1D diffusion-reaction - Multi-inputs operator

- Physics-encoded NODE:

$$\begin{cases} \dot{\psi}(t) = \sum_{i=1}^{P} W_i \odot \sigma(A_i \odot [\mathcal{P}_D \boldsymbol{D}] \odot \boldsymbol{\psi} + \boldsymbol{a}_i^1 t + B_i) + \mathcal{P}_f \boldsymbol{f}, \\ \psi(0) = \mathbf{0} \in \mathbb{R}^{d_\mathcal{U}}. \end{cases}$$

Figure: Test results of the deep NODE operator network for the learned solution operator Ψ_m^* with one random multi-input function: $\{D(x), f(x)\} \to u(x,t)$.



1D diffusion-reaction - Multi-inputs operator - Comparison

Table: Comparisons of the NODE-ONet with the MIONet for learning the solution operator with multi-input functions: $\Psi_m^\dagger : \{D(x), f(x)\} \mapsto u(t,x)$.

	Training epochs	Training resolutions	#Trainable parameters	#Training $\{D,f\}$	Test resolutions	#Test $\{D,f\}$	Absolute error	Relative error
NODE-ONet	ADAM 1×10^5	$N_x = 50$ $N_t = 10$	28,550	100	$N_x = 100$ $N_t = 100$	5,000	2.362×10^{-2}	5.297×10^{-2}
NODE-ONet	ADAM 1×10^5	$N_x = 100$ $N_t = 10$	28,550	1,000	$N_x = 100$ $N_t = 100$	5,000	4.626×10^{-3}	1.032×10^{-2}
MIONet	ADAM 1×10^5	$N_x = 100$ $N_t = 100$	161,600	100	$N_x = 100$ $N_t = 100$	5,000	1.212×10^{-1}	2.661×10^{-1}
MIONet	ADAM 1×10^5	$N_x = 100$ $N_t = 100$	161,600	1,000	$N_x = 100$ $N_t = 100$	5,000	9.491×10^{-3}	2.072×10^{-2}

1D diffusion-reaction - Prediction

Table: Prediction results of for $t \in [0,2]$. $\Psi_f^* : f(x) \mapsto u(x,t)$: the learned source-to-solution operator ,$\Psi_m^* : \{D(x), f(x)\} \mapsto u(x,t)$: the learned solution operator with multi-input functions.

		#Training input functions	Training time frame	Test time frame	Absolute error	Relative error
Ψ_f^*	NODE-ONet	500	$t \in [0,1]$	$t \in [0,2]$	6.839×10^{-3}	7.113×10^{-3}
	DeepONet				2.302×10^{-1}	2.360×10^{-1}
Ψ_m^*	NODE-ONet	1,000	$t \in [0,1]$	$t \in [0,2]$	1.392×10^{-2}	1.732×10^{-2}
	MIONet				1.012×10^{-1}	1.251×10^{-1}

1D diffusion-reaction - Prediction - Compare with DeepONet

Figure: Prediction of $\Psi_f^* : f \to u$ beyond $t \in [0,1]$ by NODE-ONet.

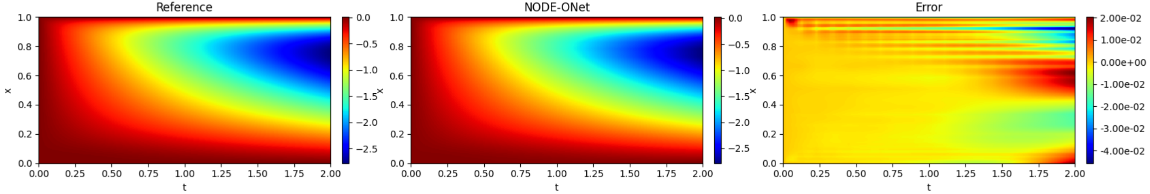
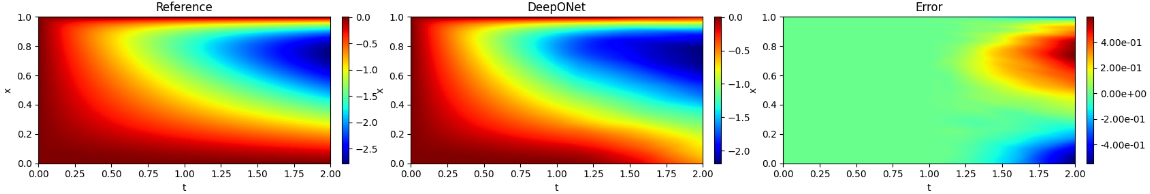


Figure: Prediction of $\Psi_f^* : f \to u$ beyond $t \in [0,1]$ by DeepONet.



1D diffusion-reaction - Prediction - Compare with MIONet

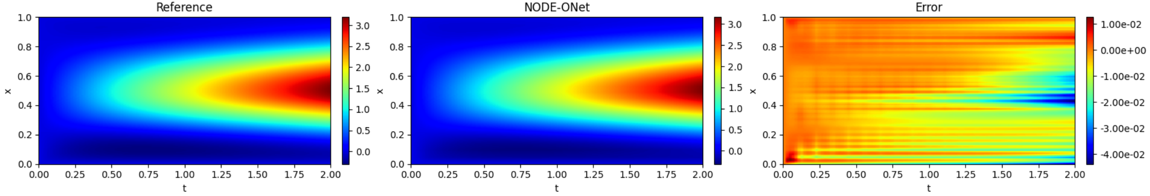


Figure: Prediction of $\Psi_m^* : \{D, f\} \to u$ beyond $t \in [0,1]$ by NODE-ONet.

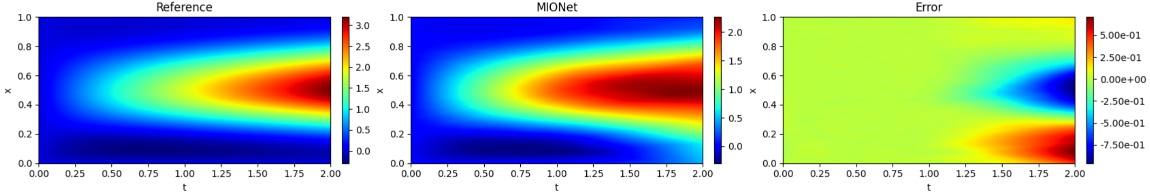


Figure: Prediction of $\Psi_m^* : \{D, f\} \to u$ beyond $t \in [0,1]$ by MIONet.

2D Navier-Stokes - Setup

We consider the following Navier-Stokes equation

$$\begin{cases} \partial_t u(t,x) + \boldsymbol{V}(t,x) \cdot \nabla u(t,x) = \nu \Delta u(t,x) + f(t,x), & \forall (t,x) \in [0,T] \times \Omega, \\ u(t,x) = \nabla \times \boldsymbol{V}(t,x) := \partial_{x_1} \boldsymbol{V}_2 - \partial_{x_2} \boldsymbol{V}_1, & \forall (t,x) \in [0,T] \times \Omega, \\ \nabla \cdot \boldsymbol{V}(t,x) = 0, & \forall (t,x) \in [0,T] \times \Omega, \\ u(0,x) = u_0(x), & \forall x \in \Omega, \end{cases}$$

with proper boundary conditions. In the following experiments, we validate the efficiency of NODE-ONets to approximate the following operators:

- Initial-to-solution operator: $u_0 \mapsto u$.
- Source-to-solution operator: $f \mapsto u$.
- Multi-inputs operator: $\{u_0, f \mapsto u\}$.

All the NODE-ONets are trained on $t \in [0, 10]$ and tested on $t \in [0, 20]$.

2D Navier-Stokes - Initial-to-solution operator

2D Navier-Stokes - Source-to-solution operator

2D Navier-Stokes - Multi-inputs operator

Outline

Conclusions

- **Theoretical Foundation:** A general error analysis for encoder-decoder networks is established, providing mathematical insights on operator approximation errors and guiding the design of NODE-ONets.
- **Physics-Encoded NODEs:** By enforcing explicit time dependence in trainable parameters and embedding PDE-specific knowledge (e.g., nonlinear dependencies and effects of known PDE parameters), these NODEs achieve superior generalization while maintaining low model complexity.
- **Numerical Efficiency:** The NODE-ONets outperform state-of-the-art methods (e.g., DeepONets, MIONet) in terms of numerical accuracy, model complexity, and training cost, especially for learning operators with multi-input functions.
- **Generalization:** Trained encoders/decoders can be transferred to related PDEs without retraining, and predictions remain satisfactory beyond the training time horizon.
- **Flexibility:** The framework accommodates various encoders/decoders (e.g., neural networks, Fourier bases) and adapts to stationary and non-stationary PDEs.

Perspectives

- **Further Error Analysis.** The error analysis in this work is mainly devoted to the generic encoder-decoder architecture. It is relevant to analyze the (approximate and generalization) errors for the NODE-ONet framework, which depends intricately on the specific PDE under consideration and is technically involved.
- **Optimal NODEs.** Note that the physics-encoded NODEs used in our experiments are not unique. Hence, it is of great theoretical and practical significance to establish a mathematical principle to determine the optimal physics-encoded NODE for a specific PDE solution operator.
- **Extensions.**
  - Extend the NODE-ONet framework to address optimal control and inverse problems involving PDEs;
  - Our current algorithm focus is on parabolic equations, developing NODE-ONets for hyperbolic equations remains crucial.

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谢谢
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ధన్యవాదాలు
Спасибо
شكرا
நன்றி
धन्यवाद
ありがとう
ขอบคุณ
감사합니다