DeepXDE: A Deep Learning Library for Solving Forward and Inverse Differential Equations

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joint work with X. Meng, Z. Mao, & G. Karniadakis

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Deep learning for partial differential equations (PDEs)

PDE-dependent approaches:

- image-like domain
  - e.g., (Long et al., *ICML*, 2018), (Zhu et al., *arXiv*, 2019)
- parabolic PDEs, e.g., through Feynman-Kac formula
  - e.g., (Beck et al., *J Nonlinear Sci*, 2017), (Han et al., *PNAS*, 2018)
- variational form
  - e.g., (E & Yu, *Commun Math Stat*, 2018)

General approaches:

- Galerkin type projection
  - e.g., (Meade & Fernandez, *Math Comput Model*, 1994), (Kharazmi et al., *arXiv*, 2019)
- strong form
  - e.g., (Dissanayake & Phan-Thien, *Commun Numer Meth En*, 1994), (Lagaris et al., *IEEE Trans Neural Netw*, 1998), (Raissi et al., *J Comput Phys*, 2019)

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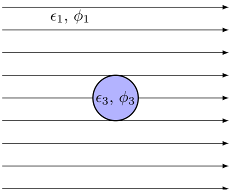
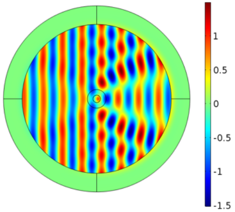
Invisible cloaking

joint work with Prof. Luca Dal Negro (Boston University)

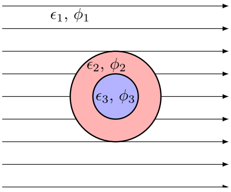
Permittivity ϵ

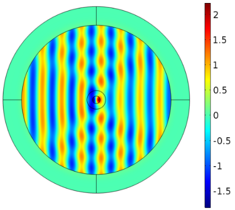
Electric field ϕ without coating





Electric field ϕ with coating

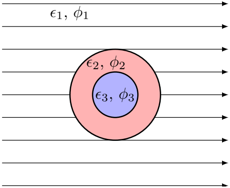




Chen, Lu, et al., *Optics Express*, submitted

Invisible cloaking

Goal: Given ϵ_1 and ϵ_3, find $\epsilon_2(x, y)$ s.t. ϕ_1 unperturbed, i.e., $\phi_1 \approx \phi_{1,target}$



Helmholtz equation ($k = \frac{2\pi}{\lambda}$)

$$\nabla^2 \phi_i + \epsilon_i k^2 \phi_i = 0, \qquad i = 1, 2, 3$$

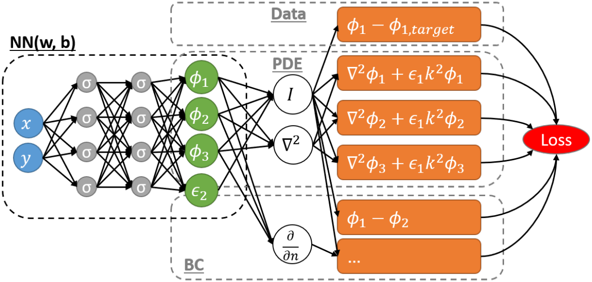
Boundary conditions:

- Outer circle: $\phi_1 = \phi_2$, $\epsilon_1 \frac{\partial \phi_1}{\partial \mathbf{n}} = \epsilon_2 \frac{\partial \phi_2}{\partial \mathbf{n}}$
- Inner circle: $\phi_2 = \phi_3$, $\epsilon_2 \frac{\partial \phi_2}{\partial \mathbf{n}} = \epsilon_3 \frac{\partial \phi_3}{\partial \mathbf{n}}$

Chen, Lu, et al., *Optics Express*, submitted

Physics-informed neural networks (PINNs)

Idea: Embed a PDE into the loss of the neural network



- mesh-free & particle-free
- inverse problems: seamlessly integrate data and physics
- black-box or noisy IC/BC/forcing terms (Pang*, Lu*, et al., *SIAM J Sci Comput*, 2019)
- a unified framework: PDE, integro-differential equations (Lu et al., *SIAM Rev*, submitted), fractional PDE (Pang*, Lu*, et al., *SIAM J Sci Comput*, 2019), stochastic PDE (Zhang, Lu, et al., *J Comput Phys*, 2019)

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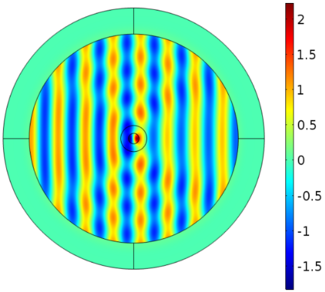
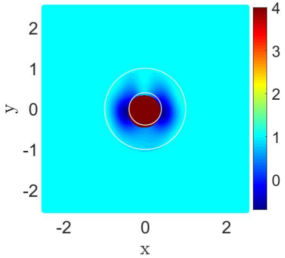
Invisible cloaking

Electric field ϕ_i



Permittivity ϵ_i



Chen, Lu, et al., *Optics Express*, submitted

Approximation: Loss $\to$ 0?

Theorem (Universal approximation theorem; Cybenko, 1989)

Let σ *be any continuous sigmoidal function. Then finite sums of the form* $G(x) = \sum_{j=1}^{N} \alpha_j \sigma(y_j \cdot x + \theta_j)$ *are dense in* $C(I_d)$.

Theorem (Pinkus, 1999)

Let $\mathbf{m}^i \in \mathbb{Z}_+^d$, $i = 1, \ldots, s$, *and set* $m = \max_{i=1,\ldots,s} |\mathbf{m}^i|$. *Assume* $\sigma \in C^m(\mathbb{R})$ *and* σ *is not a polynomial. Then the space of single hidden layer neural nets*

$$\mathcal{M}(\sigma) := span\{\sigma(\mathbf{w} \cdot \mathbf{x} + b) : \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$$

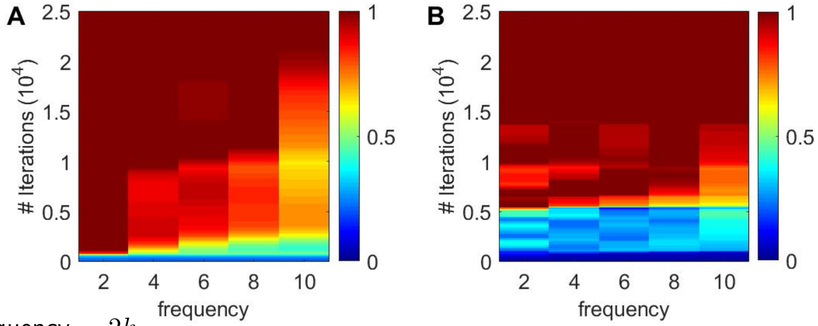
is dense in

$$C^{\mathbf{m}^1,\ldots,\mathbf{m}^s}(\mathbb{R}^d) := \cap_{i=1}^{s} C^{\mathbf{m}^i}(\mathbb{R}^d).$$

Lu et al., *SIAM Rev*, submitted

Optimization

- A: approximate $f(x) = \sum_{k=1}^{5} \sin(2kx)/(2k)$
  - learn from low to high frequencies
- B: solve the Poisson equation $-f_{xx} = \sum_{k=1}^{5} 2k \sin(2kx)$
  - all frequencies are learned almost simultaneously
  - faster learning



Frequency $= 2k$

Lu et al., *SIAM Rev*, submitted

Generalization: Residual-based adaptive refinement (RAR)

Challenge: Uniform residual points are not efficient for PDEs with steep solutions.
e.g., Burgers equation ($x \in [-1, 1],\ t \in [0, 1]$):

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}, \quad u(x, 0) = -\sin(\pi x), \quad u(-1, t) = u(1, t) = 0.$$

Lu et al., *SIAM Rev*, submitted

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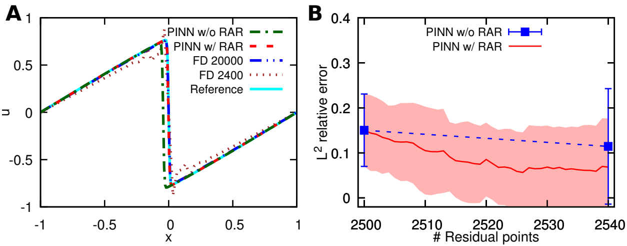
- Idea: adaptively add more points in locations with large PDE residual $\left\| f\left(\mathbf{x}; \frac{\partial \hat{u}}{\partial x_1}, \ldots, \frac{\partial \hat{u}}{\partial x_d}; \frac{\partial^2 \hat{u}}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 \hat{u}}{\partial x_1 \partial x_d}; \ldots; \boldsymbol{\lambda}\right)\right\|$

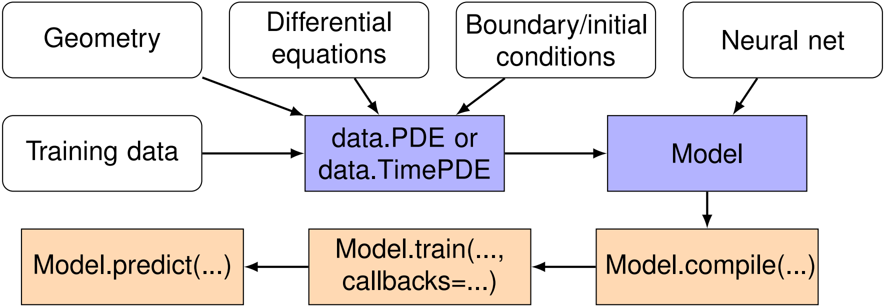


10,000 (Raissi et al., *J Comput Phys*, 2019) ↓ 2,540

Lu et al., *SIAM Rev*, submitted

Usage of DeepXDE

Solving differential equations in DeepXDE is no more than specifying the problem using the build-in modules



Poisson equation

2D Poisson equation over an L-shaped domain $\Omega = [-1, 1]^2 \setminus [0, 1]^2$:

$$-\Delta u(x, y) = 1, \quad (x, y) \in \Omega, \qquad u(x, y) = 0, \quad (x, y) \in \partial\Omega.$$

1. geometry

```
geom = dde.geometry.Polygon(
    [[0, 0], [1, 0], [1, -1], [-1, -1], [-1, 1], [0, 1]])
```

2. PDE or PDE system

```
def pde(x, y):
    dy_x = tf.gradients(y, x)[0]
    dy_x, dy_y = dy_x[:, 0:1], dy_x[:, 1:]
    dy_xx = tf.gradients(dy_x, x)[0][:, 0:1]
    dy_yy = tf.gradients(dy_y, x)[0][:, 1:]
    return -dy_xx - dy_yy - 1
```

3. BC: Dirichlet, Neumann, Robin, periodic, and a general BC

```
def boundary(x, on_boundary):
    return on_boundary
def func(x):
    return np.zeros([len(x), 1])

bc = dde.DirichletBC(geom, func, boundary)
```

Poisson equation

4. "data": geometry + PDE + BC + "training" points

```
data = dde.data.PDE(
    geom, 1, pde, bc, num_domain=1200, num_boundary=120)
```

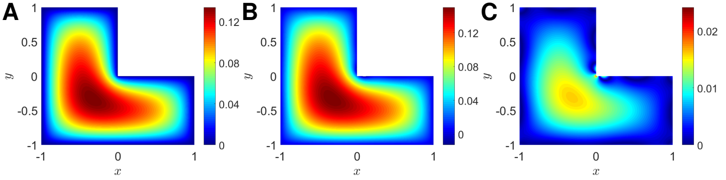
5. network: feed-forward network, or residual network

```
net = dde.maps.FNN([2]+[50]*4+[1], "tanh", "Glorot uniform")
```

6. model: data + network, and train

```
model = dde.Model(data, net)
model.compile("adam", lr=0.001)
model.train(epochs=50000)
```

(A) spectral element, (B) PINN, (C) error



Diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 x}{\partial x^2} - e^{-t}(1 - \pi^2)\sin(\pi x), \quad x \in [-1, 1], t \in [0, 1]$$

with Dirichlet BC. (Exact solution $u(x, t) = e^{-t}\sin(\pi x)$)

- geometry

```
geom = dde.geometry.Interval(-1, 1)
timedomain = dde.geometry.TimeDomain(0, 1)
geomtime = dde.geometry.GeometryXTime(geom, timedomain)
```

- IC, similar to Dirichlet BC

```
def func(x):
    return np.sin(np.pi * x[:, 0:1]) * np.exp(-x[:, 1:])

ic = dde.IC(geomtime, func, lambda _, on_initial: on_initial)
```

Inverse problem

A diffusion-reaction system on $x \in [0, 1], t \in [0, 10]$:

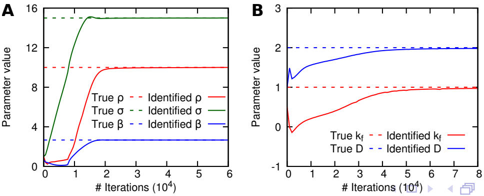
$$\frac{\partial C_A}{\partial t} = D\frac{\partial^2 C_A}{\partial x^2} - k_f C_A C_B^2, \quad \frac{\partial C_B}{\partial t} = D\frac{\partial^2 C_B}{\partial x^2} - 2k_f C_A C_B^2$$

- Define D and k_f as trainable variables

```
kf = tf.Variable(0.05)
D = tf.Variable(1.0)
```

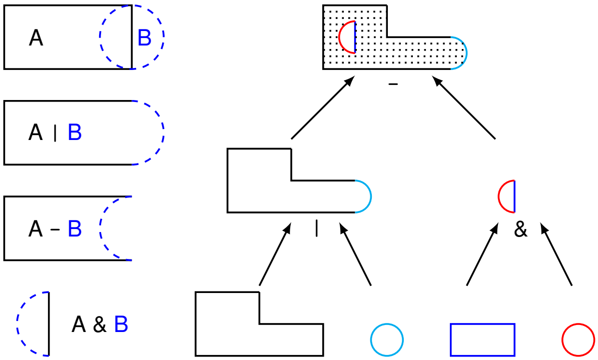
- Define C_A measurements as DirichletBC (the same for C_B)

```
observe_x = ...  # All the locations of measurements
observe_Ca = ...  # The corresponding measurements of Ca
ptset = dde.bc.PointSet(observe_x)
observe = dde.DirichletBC(geomtime, ptset.values_to_func(
    observe_Ca), lambda x, _: ptset.inside(x), component=0)
```



Constructive solid geometry

- Primitive geometries
  - **`interval`**, **`triangle`**, **`rectangle`**, **`polygon`**, **`disk`**, **`cuboid`**, **`sphere`**
- boolean operations:
  - Union $A|B$
  - difference $A - B$
  - intersection $A\&B$



DeepXDE

Installation

- `pip install deepxde`
- `conda install -c conda-forge deepxde`

`https://github.com/lululxvi/deepxde`

- Well-structured and highly configurable. All the components are loosely coupled.

Thank you!