DeepONet: Learning nonlinear operators

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From function to operator

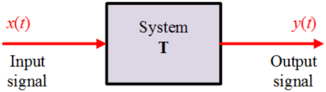
- Function: $\mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$

  e.g., image classification:  $\mapsto$ 5

- Operator: function (∞-dim) $\mapsto$ function (∞-dim)

  e.g., derivative (local): $x(t) \mapsto x'(t)$

  e.g., integral (global): $x(t) \mapsto \int K(s,t)x(s)ds$

  e.g., dynamic system: 

  e.g., biological system

  e.g., social system

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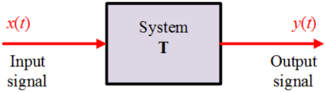

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  $\Rightarrow$ Can we learn operators via neural networks?

  $\Rightarrow$ How?

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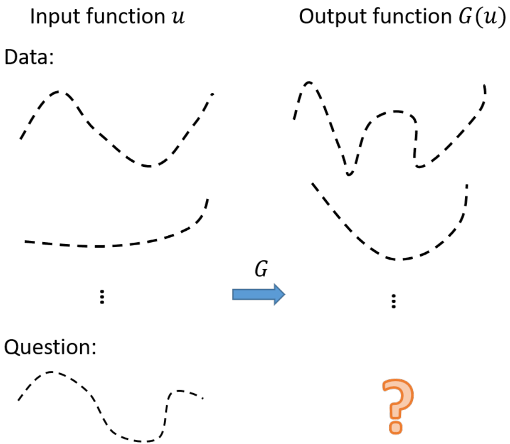
Problem setup

$G : u \mapsto G(u)$
$G(u) : y \in \mathbb{R}^d \mapsto G(u)(y) \in \mathbb{R}$



Universal Approximation Theorem for Operator

$G : u \mapsto G(u)$
$G(u) : y \in \mathbb{R}^d \mapsto G(u)(y) \in \mathbb{R}$

Theorem (Chen & Chen, 1995)

Suppose that σ is a continuous non-polynomial function, X is a Banach Space, $K_1 \subset X$, $K_2 \subset \mathbb{R}^d$ are two compact sets in X and $\mathbb{R}^d$, respectively, V is a compact set in $C(K_1)$, G is a continuous operator, which maps V into $C(K_2)$. Then for any $\epsilon > 0$, there are positive integers n, p, m, constants $c_i^k, \xi_{ij}^k, \theta_i^k, \zeta_k \in \mathbb{R}$, $w_k \in \mathbb{R}^d$, $x_j \in K_1$, $i = 1, \ldots, n$, $k = 1, \ldots, p$, $j = 1, \ldots, m$, such that

$$\left| G(u)(y) - \sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k u(x_j) + \theta_i^k \right) \sigma(w_k \cdot y + \zeta_k) \right| < \epsilon$$

holds for all $u \in V$ and $y \in K_2$.

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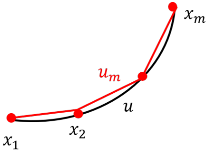
Convergence w.r.t. the number of sensors

Consider $G : u(x) \mapsto \boldsymbol{s}(x)$ ($x \in [0,1]$) by ODE system

$$\frac{d}{dx}\boldsymbol{s}(x) = \boldsymbol{g}(\boldsymbol{s}(x), u(x), x), \quad \boldsymbol{s}(0) = \boldsymbol{s_0}$$

$\forall u \in V \Rightarrow u_m \in V_m$



Let $\kappa(m, V) := \sup_{u \in V} \max_{x \in [0,1]} |u(x) - u_m(x)|$

e.g., Gaussian process with kernel $e^{-\frac{\|x_1 - x_2\|^2}{2l^2}}$: $\kappa(m, V) \sim \frac{1}{m^2 l^2}$

Theorem (Lu et al., 2019; informal)

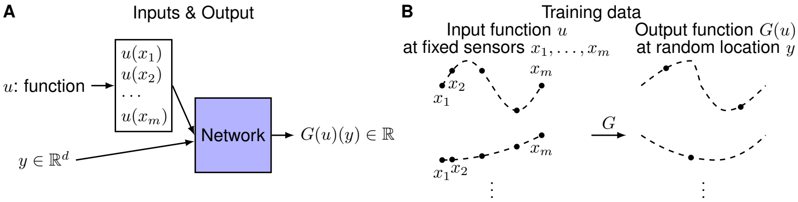
There exists a constant C, such that for any $y \in [0,1]$,

$$\sup_{u \in V} \|G(u)(y) - NN(u(x_1), \ldots, u(x_m), y)\|_2 < C\kappa(m, V).$$

Problem setup

$G : u \mapsto G(u)$
$G(u) : y \in \mathbb{R}^d \mapsto G(u)(y) \in \mathbb{R}$

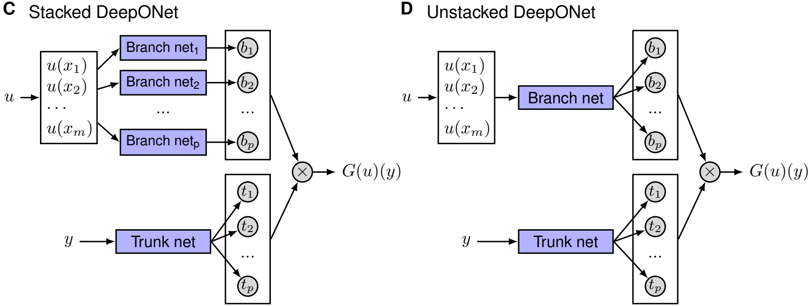
- Inputs: u at sensors $\{x_1, x_2, \ldots, x_m\}$, $y \in \mathbb{R}^d$
- Output: $G(u)(y) \in \mathbb{R}$



Next, how to design the network?

Lu et al., arXiv:1910.03193, 2019

Deep operator network (DeepONet)



$$G(u)(y) \approx \sum_{k=1}^{p} b_k(u) \cdot t_k(y)$$

Ideas:

- Prior knowledge: u and y are independent
- $G(u)(y)$: a function of y conditioning on u
  - $t_k(y)$: basis functions of y
  - $b_k(u)$: u-dependent coefficients

Lu et al., arXiv:1910.03193, 2019

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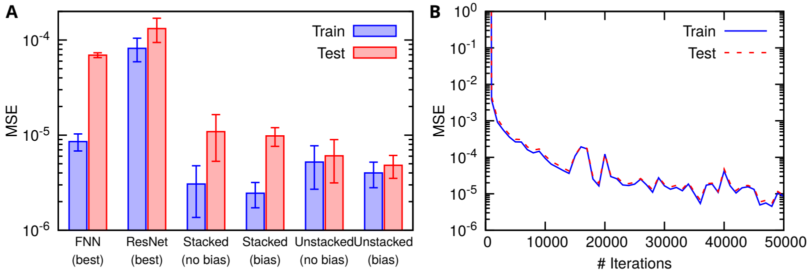
Explicit operator: A simple ODE case

$$\frac{ds(x)}{dx} = u(x), \quad x \in [0,1], \quad s(0) = 0$$

$$G : u(x) \mapsto s(y) = s(0) + \int_0^y u(\tau) d\tau$$

Very small generalization error!

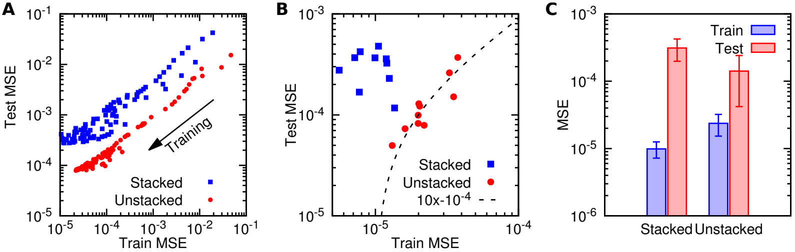


More problems: 1D Caputo fractional derivative, 2D Riesz fractional Laplacian

Lu et al., arXiv:1910.03193, 2019

Implicit operator: A nonlinear ODE case

$$\frac{ds(x)}{dx} = -s^2(x) + u(x)$$



Linear correlation between training and test errors

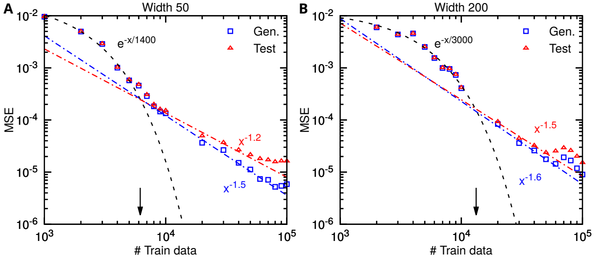
- A: in one training process
- B: across multiple runs (random dataset and network initialization)

Lu et al., arXiv:1910.03193, 2019

Implicit operator: Gravity pendulum with an external force

$$\frac{ds_1}{dt} = s_2, \qquad \frac{ds_2}{dt} = -k \sin s_1 + u(t)$$

$G : u(x) \mapsto \mathbf{s}(x)$



Test/generalization error:

- small dataset: exponential convergence
- large dataset: polynomial rates
- larger network has later transition point

Lu et al., arXiv:1910.03193, 2019

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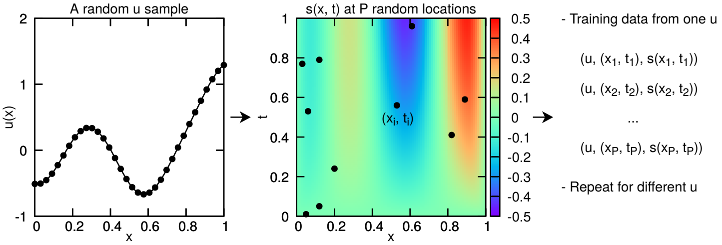
Implicit operator: Diffusion-reaction system

$$\frac{\partial s}{\partial t} = D\frac{\partial^2 s}{\partial x^2} + ks^2 + u(x), \quad x \in [0,1], t \in [0,1]$$



$\#$ Training points $= \#u \times P$

Lu et al., arXiv:1910.03193, 2019

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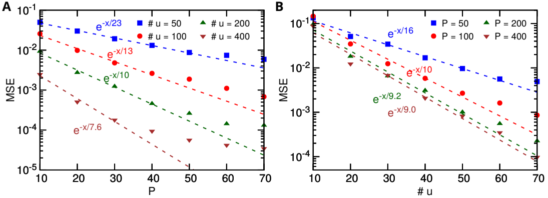
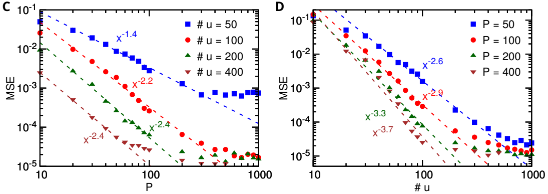
Small dataset: Exponential convergence



Large dataset: Polynomial convergence



Lu et al., arXiv:1910.03193, 2019

Advection-diffusion system

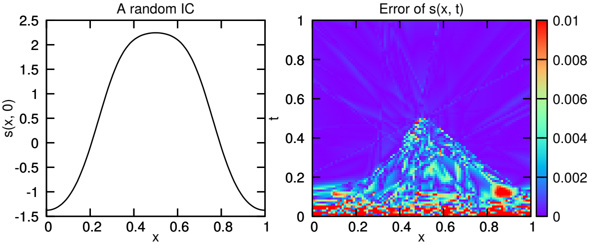
$$\frac{\partial s}{\partial t} + \frac{\partial s}{\partial x} - \frac{\partial^2 s}{\partial x^2} = 0 \quad \text{or} \quad \frac{\partial s}{\partial t} - 1.5({}^{RL}_{-\infty}D_x^{1.5})s = 0$$

$x \in [0,1]$, $t \in [0,1]$, periodic BC

$G : u(x) = s(x,0) \mapsto s(x,t)$

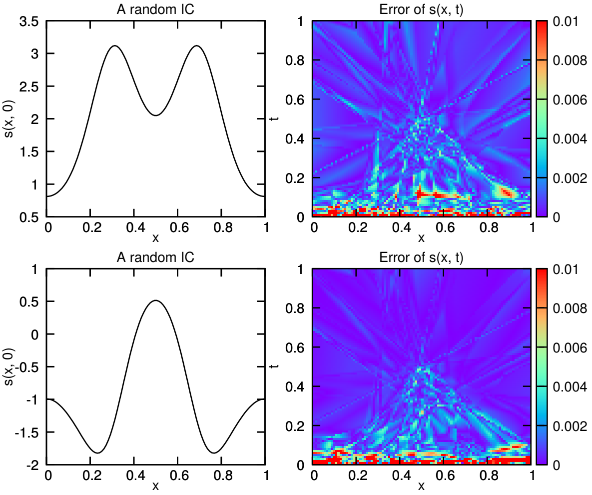
- 100 u sensors
- training data: # IC = 1000, 100 random points of $s(x,t)$ for each IC

Prediction for a new random IC:



Advection-diffusion system

More predictions:



Stochastic ODE

Consider the population growth model

$$dy(t;\omega) = k(t;\omega)y(t;\omega)dt, \quad y(0) = 1$$

Stochastic process $k(t;\omega) \sim \mathcal{GP}(0, \sigma^2 \exp(-\|t_1 - t_2\|^2/2l^2))$

Goal: Given a *new* $k(t;\omega)$, predict the stochastic solution $y(t;\omega)$

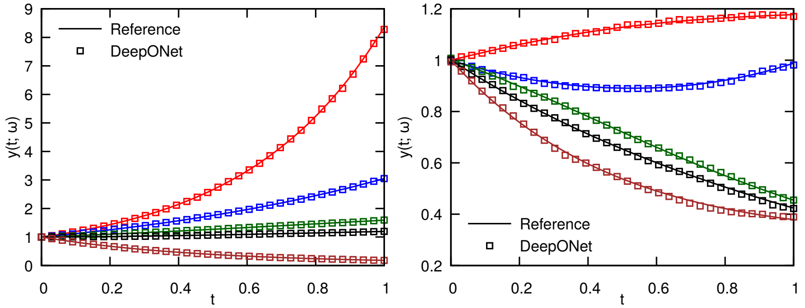
Ideas:

- Karhunen-Loève (KL) expansion: $k(t;\omega) \approx \sum_{i=1}^{N} \sqrt{\lambda_i} e_i(t)\xi_i(\omega)$
- branch net inputs: $[\sqrt{\lambda_1}e_1(t), \sqrt{\lambda_2}e_2(t), \dots, \sqrt{\lambda_N}e_N(t)] \in \mathbb{R}^{N\times m}$, where $\sqrt{\lambda_i}e_i(t) = \sqrt{\lambda_i}[(e_i(t_1), e_i(t_2)), \dots, e_i(t_m)] \in \mathbb{R}^m$
- trunk net inputs: $[t, \xi_1, \xi_2, \dots, \xi_N] \in \mathbb{R}^{N+1}$

Stochastic ODE

- Choose $N = 5$ to conserve 99.9% stochastic energy
- Train with 10000 different $k(t;\omega)$ with l randomly sampled in $[1, 2]$, and for each $k(t;\omega)$ we use only one realization
- Test MSE is $8.0 \times 10^{-5} \pm 3.4 \times 10^{-5}$

Example: 10 different random samples from $k(t;\omega)$ with $l = 1.5$

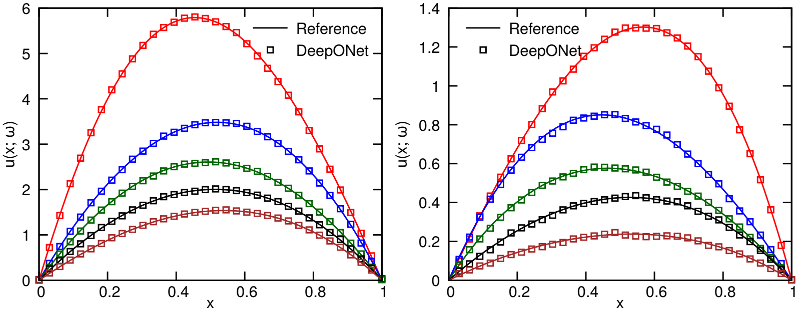


Stochastic PDE

Consider the elliptic problem with multiplicative noise

$$-\mathrm{div}(e^{b(x;\omega)}\nabla u(x;\omega)) = f(x), \quad x \in (0,1)$$

with zero Dirichlet boundary conditions, $f(x) = 10$.
Stochastic process $b(x;\omega) \sim \mathcal{GP}(0, \sigma^2 \exp(-\|x_1 - x_2\|^2/2l^2))$



DeepONet

Diverse applications:

- Explicit operators: integral operators, fractional derivative, fractional Laplacian
- Implicit operators: (linear or nonlinear) ODE/PDE system, stochastic ODE/PDE

Good performance & data efficiency:

- Small generalization error
- Exponential/polynomial error convergence