DeepONet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators

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Introduction

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

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

  $\Rightarrow$ Neural network [Universal approximation theorem]

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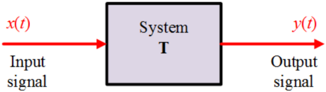
  e.g., integral (global): $x(t) \mapsto \int K(s,t)x(s)ds$

  e.g., dynamic system: 

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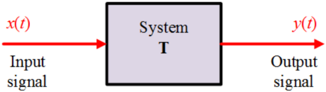
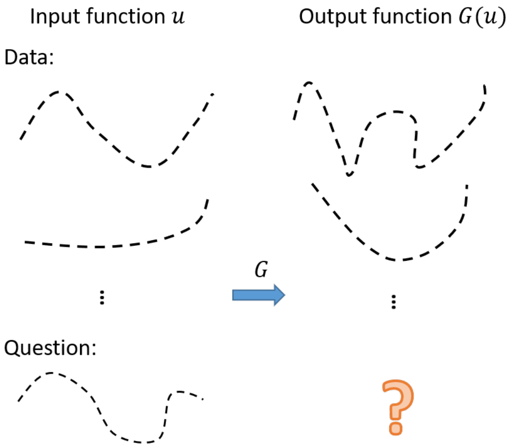
  e.g., dynamic system: 

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

Problem setup

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



Network inputs and output

$G : u \mapsto G(u)$
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- Inputs: u (∞-dim?), $y \in \mathbb{R}^d$
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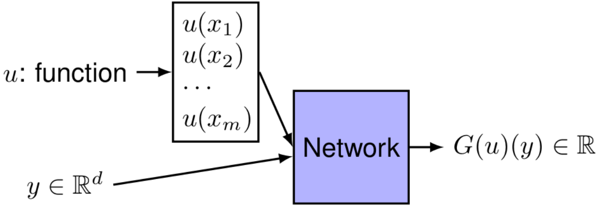

Assume $\{x_i\}$ “dense” enough,
is there a universal approximation theorem for operator?

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, IEEE Trans. Neural Netw., 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 nonlinear continuous operator, which maps V into $C(K_2)$. Then for any $\epsilon > 0$, there are positive integers n, p, m, constants $c_i^k, \xi_{ij}^k, \theta_i^k, \zeta_k \in \mathbb{R}$, $w_k \in \mathbb{R}^d$, $x_j \in K_1$, $i = 1, \dots, n$, $k = 1, \dots, p$, $j = 1, \dots, m$, 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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Number of sensors

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

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

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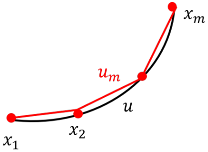

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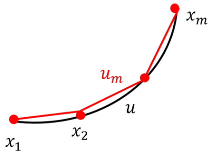

Let $\kappa(m, V) := \sup_{u \in V} \max_{x \in [0,1]} |u(x) - u_m(x)|$

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

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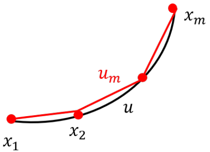

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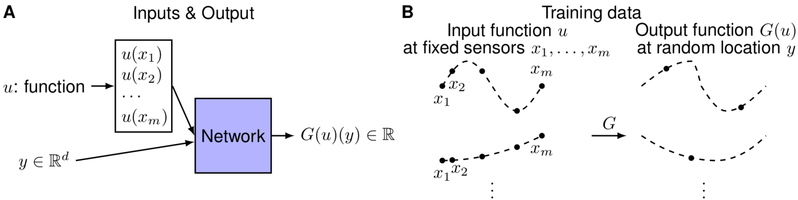
Theorem (informal)

There exists a constant C, such that for any y,

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

So far, we show

- operators can be approximated by neural networks
- the number of sensors we need



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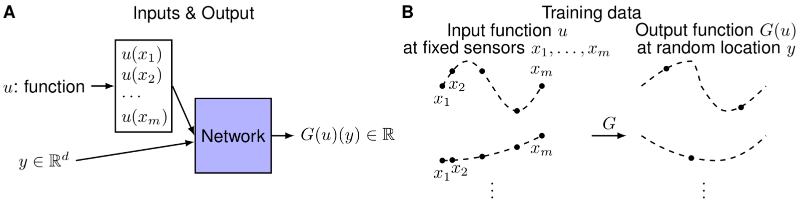


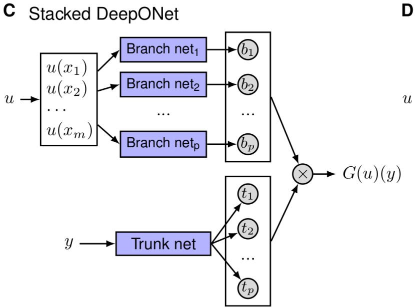
Q: How to design the network?

$\Rightarrow$ Deep operator network (DeepONet)

DeepONet

Recall the Theorem:

$$G(u)(y) \approx \sum_{k=1}^{p} \underbrace{\sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k u(x_j) + \theta_i^k \right)}_{branch} \underbrace{\sigma(w_k \cdot y + \zeta_k)}_{trunk}$$



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A simple ODE case

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

with an initial condition $s(0) = 0$.

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

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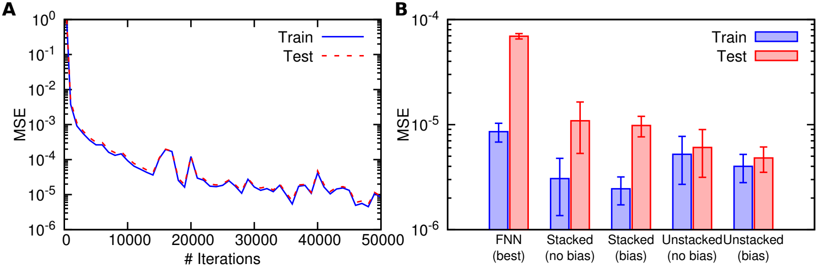
100 u sensors, 10000×1 training points
Very small generalization error!



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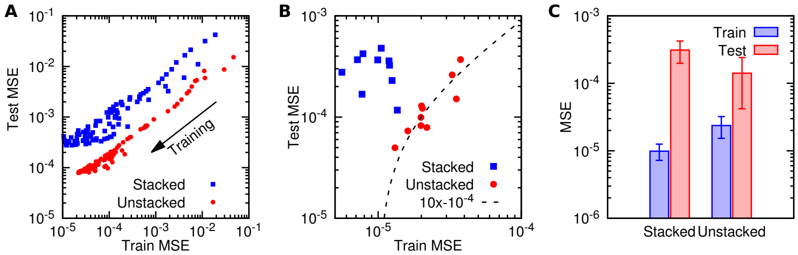

Linear correlation between training and test errors

- A: in one training process

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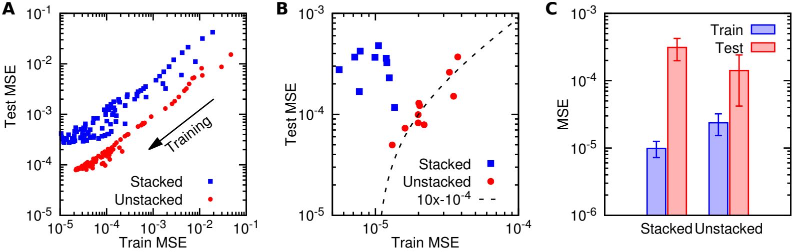
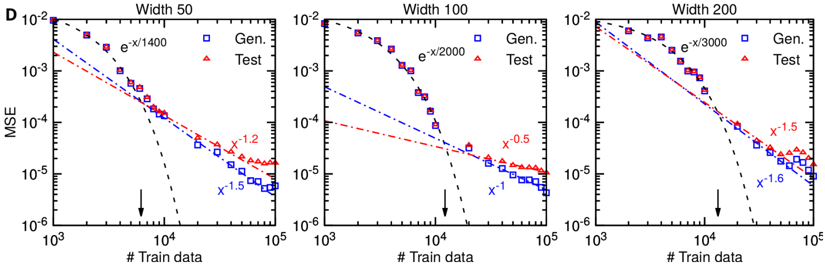


Linear correlation between training and test errors

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

Gravity pendulum with an external force $u(t)$

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

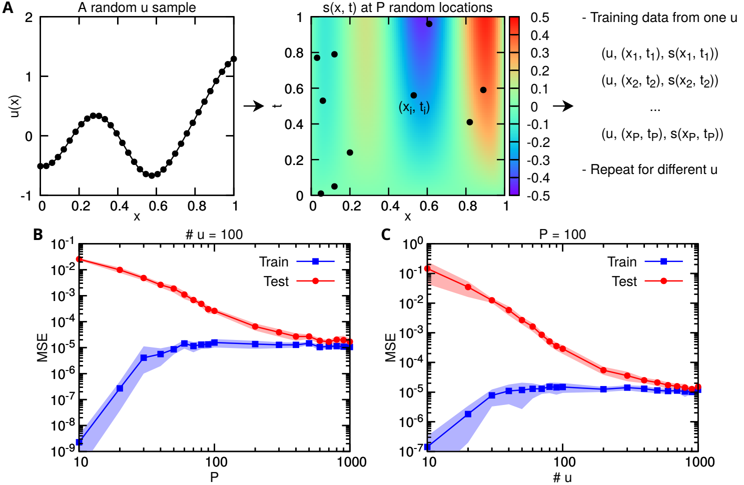


Test/generalization error:

- small dataset: exponential convergence
- large dataset: polynomial rates
- smaller network has earlier transition point

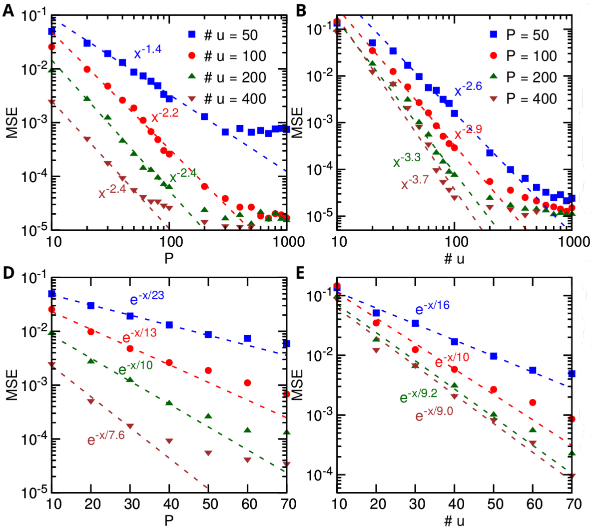
Diffusion-reaction system

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



Diffusion-reaction system

exponential/polynomial convergence



Summary

- Number of sensors, $\kappa(m, V)$
- DeepONet
  - 1D ODE (linear, nonlinear), gravity pendulum, diffusion-reaction system (nonlinear)
  - Small generalization error
  - Exponential/polynomial error convergence

- Lu, Jin, & Karniadakis, arXiv:1910.03193, 2019.
- DeepXDE: `https://deepxde.rtfd.io`

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