NEURAL OPERATORS FOR SCIENTIFIC MACHINE LEARNING

Presented by Handi Zhang

Functions map data, Operators map functions

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

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

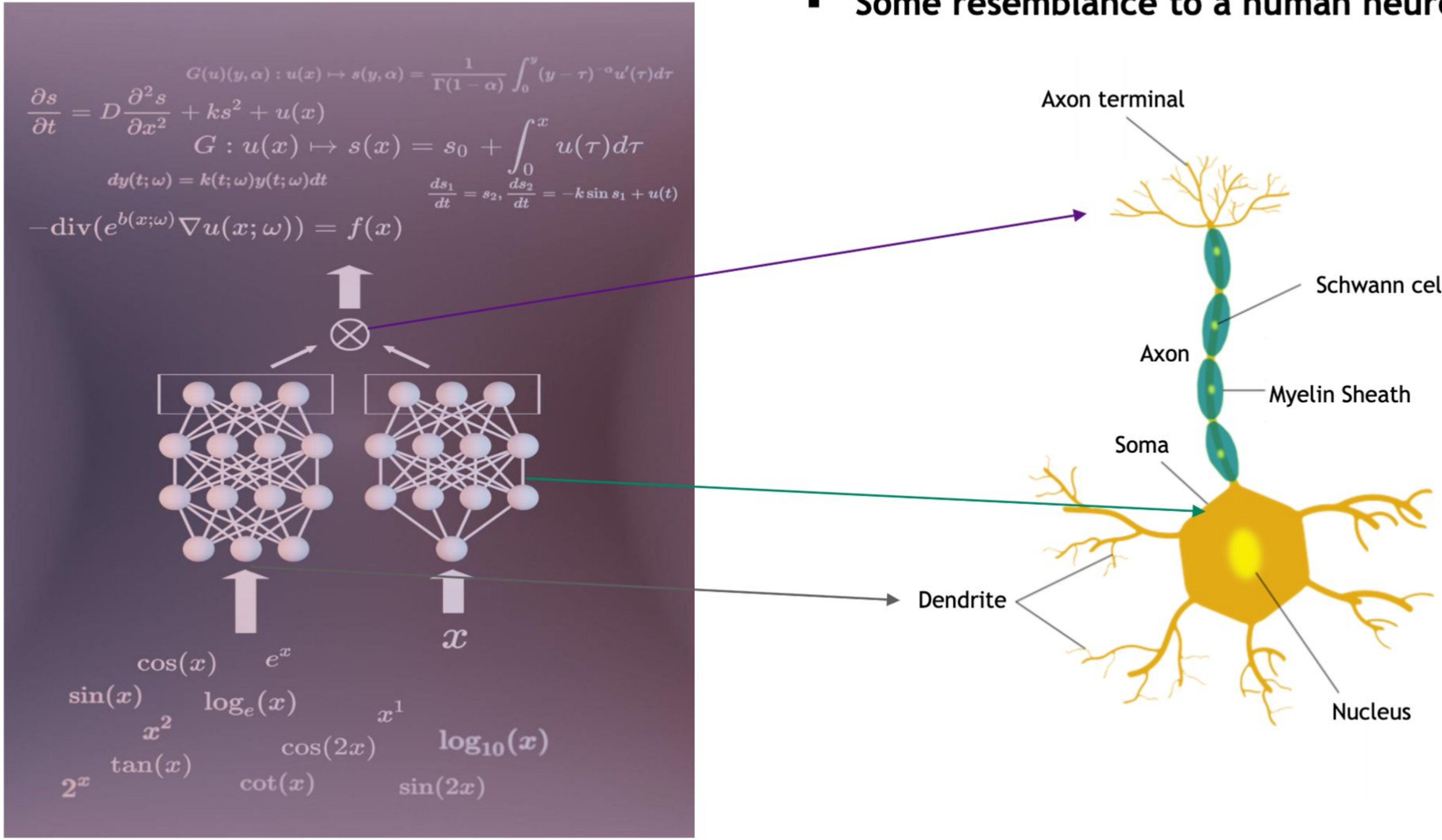
- Operator: function (∞-dim) $\mapsto$ function (∞-dim)
  e.g., derivative (local): $x(t) \mapsto x'(t)$
  e.g., integral (global): $x(t) \mapsto \int K(s,t)x(s)ds$

  e.g., dynamic system: $x(t)$  $y(t)$

  e.g., biological system
  e.g., social system

Deep Operator Network (DeepONet)

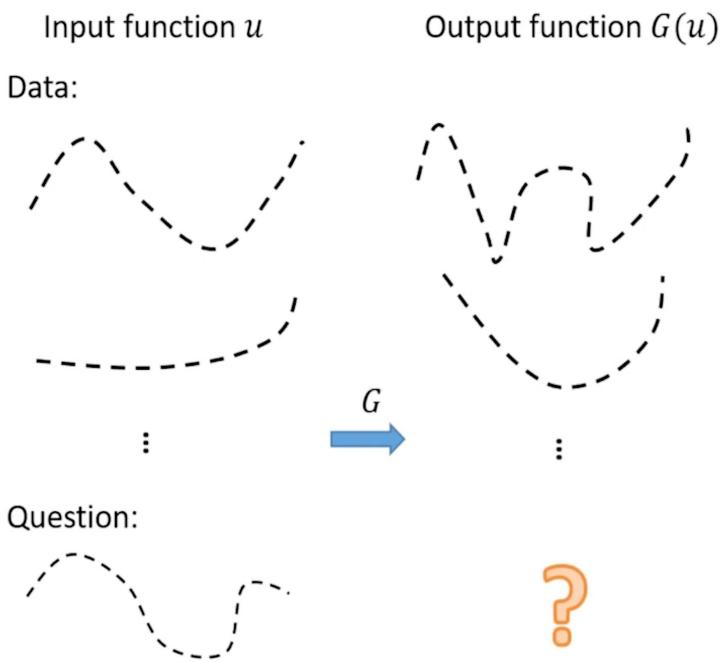
- **Some resemblance to a human neuron**

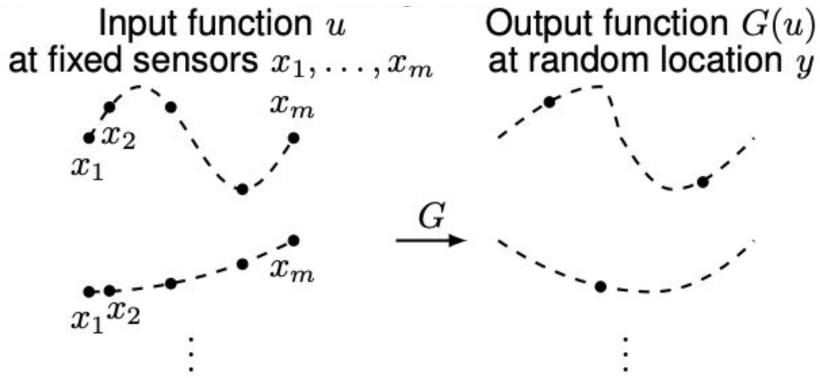


Problem Setup

$G : u \mapsto G(u)$

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





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

- Inputs: u at sensors $\{x_1, x_2, \ldots, x_m\}, y$
- Outputs: $G(u)(y)$
- $G(u)(y)$: a function of y conditioning on u
  - $t_k(y)$: basis functions of y
  - $b_k(u)$: u-dependent coefficient

Universal Approximation Theorem for Operator

Theorem 1 (Universal Approximation Theorem for Operator). *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 and m, constants c_i^k, ξ_{ij}^k, θ_i^k, $\zeta_k \in \mathbb{R}$, $w_k \in \mathbb{R}^d$, $x_j \in K_1$, $i = 1, \dots, n$, $k = 1, \dots, p$ and $j = 1, \dots, m$, such that*

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

holds for all $u \in V$ and $y \in K_2$. Here, $C(K)$ is the Banach space of all continuous functions defined on K with norm $\| f \|_{C(K)} = \max_{x \in K} |f(x)|$.

Generalized Universal Approximation Theorem for Operator

Theorem 2 (Generalized Universal Approximation Theorem for Operator). *Suppose that 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 $C(K_1)$. Assume that $G: V \to C(K_2)$ is a nonlinear continuous operator. Then, for any $\epsilon > 0$, there exist positive integers m, p, continuous vector functions $\mathbf{g} : \mathbb{R}^m \to \mathbb{R}^p$, $\mathbf{f} : \mathbb{R}^d \to \mathbb{R}^p$, and $x_1, x_2, \ldots, x_m \in K_1$, such that*

$$\left| G(u)(y) - \langle \underbrace{\mathbf{g}(u(x_1), u(x_2), \cdots, u(x_m))}_{\text{branch}}, \underbrace{\mathbf{f}(y)}_{\text{trunk}} \rangle \right| < \epsilon$$

holds for all $u \in V$ and $y \in K_2$, where $\langle \cdot, \cdot \rangle$ denotes the dot product in $\mathbb{R}^p$. Furthermore, the functions $\mathbf{g}$ and $\mathbf{f}$ can be chosen as diverse classes of neural networks, which satisfy the classical universal approximation theorem of functions, for example, (stacked/unstacked) fully connected neural networks, residual neural networks and convolutional neural networks.

Sketch of Proof

Continuously extend $\mathcal{G}(u)(y), y \in K_2$ to $\mathcal{G}(u)(y), y \in D$.

$$
\begin{aligned}
\mathcal{G}(u) &\approx \mathcal{G}(\mathcal{I}^0_{m,x} u) \quad \text{(piecewise constant interpolation)} \\
&\approx \sum_{k=1}^{p} \int_D \mathcal{G}(\mathcal{I}^0_{m,x} u) e_k(y) dy \; e_k(y), \quad (K_2 \subset D, \text{spectral expansion}) \\
&\approx \sum_{k=1}^{p} \int_D \mathcal{I}^0_{n,y}(\mathcal{G}(\mathcal{I}^0_{m,x} u)(y)) e_k(y) dy e_k(y) \quad \text{(interpolation)} \\
&= \sum_{k=1}^{p} (\sum_{i=1}^{n} \mathcal{G}(\mathcal{I}^0_{m,x} u)(y_i) \underbrace{\int_D e_k(y) \chi_{D_i}(y) dy}_{c_i^k}) e_k(y)
\end{aligned}
$$

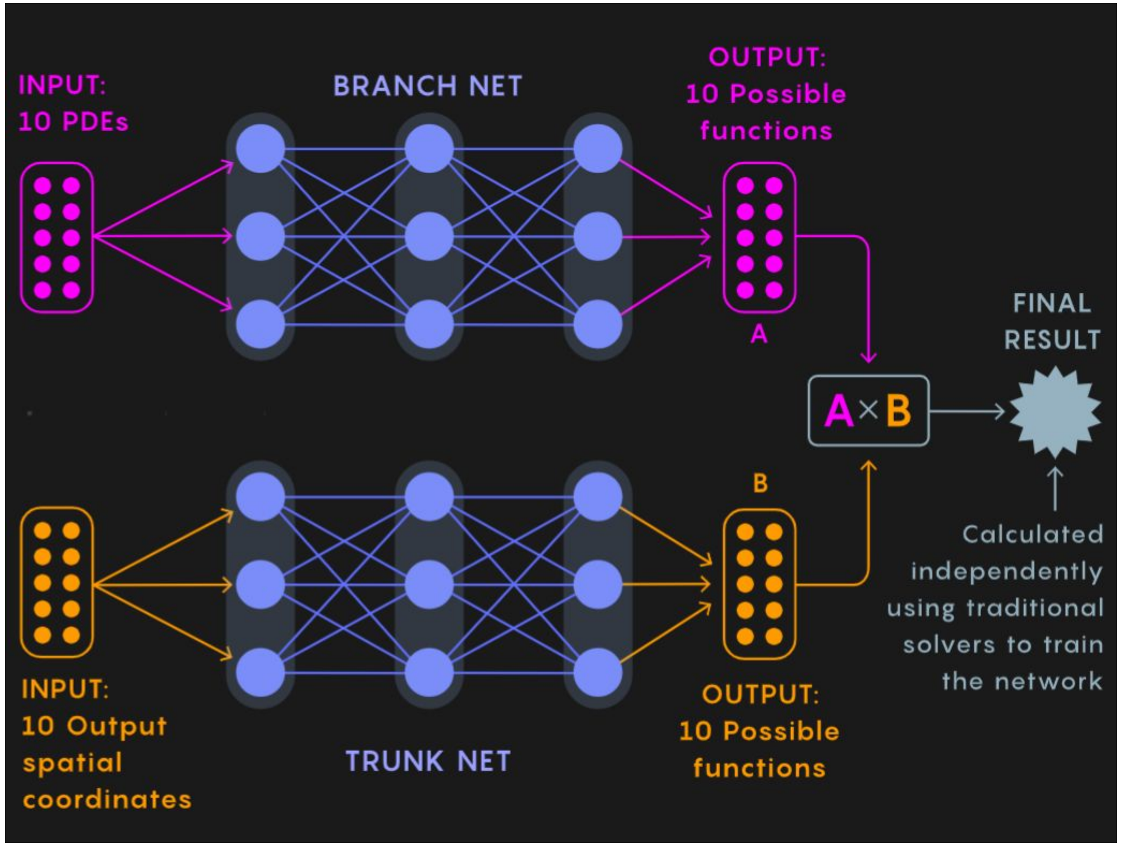
- $\mathcal{G}\left(\mathcal{I}^0_m u\right)(y_i)$ is continuous in u_m, on $[-M, M]^m$, $M = \max_{1 \le i \le m} |u(x_i)|$.
- As $\mathcal{G}: V \to C(D)$ is continuous, we have uniform approximation

$$
\sup_{u \in V} \sup_{u_m \in [-M,M]^m} \left| \mathcal{G}\left(\mathcal{I}^0_m u\right)(y_i) - g^{\mathcal{N}}\left(u_m; \Theta^{(k,i)}\right) \right| < \epsilon
$$

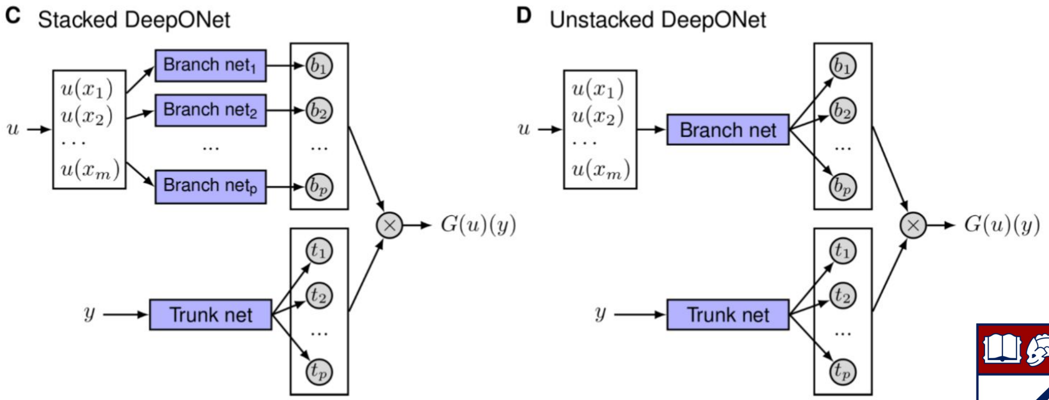
- $e_k(y) \approx f^{\mathcal{N}}\left(y; \theta^{(k)}\right)$

B. Deng, Y. Shin, L. Lu, Z. Zhang, & G. E. Karniadakis. Convergence rate of DeepONets for learning operators arising from advection-diffusion equations. arXiv preprint arXiv:2102.10621, 2021.

DeepONet



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



Error Estimates

For all the explicit and implicit operators in our examples, the operators G are Hölder continuous.

$$\|G(f) - G(g)\|_X \leq C\,\|f - g\|_Y^\alpha, \quad 0 < \alpha \leq 1.$$

Here $C > 0$ depends on f and g and the operator G. Here X and Y are Banach spaces and they refer to the space of continuous functions on a compact set unless otherwise stated.

Let $G_{\mathbb{N}}$ be the approximated G using DeepONet. Let f_h be an approximation of f in Y, possibly by collocation or neural networks. Then

$$\|G(f) - G_{\mathbb{N}}(f_h)\|_X \leq \|G(f) - G(f_h)\|_X + \|G(f_h) - G_{\mathbb{N}}(f_h)\|_X \leq C\,\|f - f_h\|_Y^\alpha + \varepsilon,$$

where ε is the user-defined accuracy as in the universal approximation theorem by neural networks and thus the key is to verify the operator G is Hölder continuous.

The explicit operators and their Lipschitz continuity ($\alpha = 1$) are presented below.

1. (Simple ODE, **Problem 1.A**) $G(u)(x) = s_0 + \int_0^x u(s)\,ds$.

$$\max_{x\in[0,b]} |G(u)(x) - G(v)(x)| \leq b \max_{x\in[0,b]} |u - v|\,.$$

2. (Caputo derivative, **Problem 2**) The operator is Lipschitz continuous with respect to its argument in weighted Sobolev norms; see e.g. [14, Theorem 2.4].

3. (Integral fractional Laplacian, **Problem 3**) The operator is Lipschitz continuous with respect to its argument in weighted Sobolev norms, see e.g. [6, Theorem 3.3].

4. (Legendre transform, **Problem 7** in Equation (S1)). The Lipschitz continuity of the operator $G(u)(n) = \int_{-1}^1 P_n(x)u(x)\,dx$ can be seen as follows. For any non-egative integer,

$$\max_n |G(u)(n) - G(v)(n)| \leq \max_n \int_{-1}^1 |P_n(x)|\,dx \max_{x\in[-1,1]} |u - v| \leq C \max_{x\in[-1,1]} |u - v|$$

   where $C = \max_n \left(\int_{-1}^1 dx\right)^{1/2}\left(\int_{-1}^1 |P_n(x)|^2\,dx\right)^{1/2} = \max_n (2\frac{2}{2n+1})^{1/2} \leq 2$.

5. The linear operator from **Problem 9** in (S2) in Lipschitz continuous with respect to the initial condition in the norm in the space of continuous functions, from he classical theory for linear parabolic equations [9, Chapter IV],

The implicit operator from **Problem 6**. The operator can be written as $u = G(b)$ and $u_i = G(b_i)$, $i = 1, 2$ satisfying the following equations:

$$-\mathrm{div}(e^{b_i(x)}\nabla u_i) = f(x), \quad x \in D = (0,1), \qquad u_i(x) = 0, \quad x \in \partial D,$$

Then $\|u_i(\omega)\|_{H^1} \leq (\min_{x\in D} e^{-b_i})^{-1}\,\|f\|_{H^{-1}}$, where H^1 and H^{-1} are standard Sobolev-Hilbert spaces. The difference $u_1 - u_2$ satisfies the following

$$-\mathrm{div}(e^{b_1(x)}\nabla(u_1 - u_2)) = \mathrm{div}((e^{b_1(x)} - e^{b_2(x)})\nabla u_2), \quad x \in D, \qquad u_1 - u_2 = 0, \quad x \in \partial D.$$

Then by the stability of the elliptic equation , we have

$$\begin{aligned}
\|u_1(\omega) - u_2(\omega)\|_{H^1} &\leq (\min_{x\in D} e^{b_i(x)})^{-1} \left\|(e^{b_1} - e^{b_2})\nabla u_2\right\|_{L^2} \\
&= (\min_{x\in D} e^{b_1(x)})^{-1} \left\|e^{b_1} - e^{b_2}\right\|_{C(D)} \|u_2\|_{H^1} \\
&\leq (\min_{x\in D} e^{b_1(x)})^{-1}(\min_{x\in D} e^{b_2(x)})^{-1} \left\|e^{b_1} - e^{b_2}\right\|_{C(D)} \|f\|_{H^{-1}}\,.
\end{aligned}$$

Then by the mean value theorem, $|e^x - e^y| \leq |x - y|\,(e^x + e^y)$ holds for all $x, y \in \mathbb{R}$. Thus,

$$\|u_1(\omega) - u_2(\omega)\|_{H_0^1} \leq (\min_{x\in D} e^{b_1(x)})^{-1}(\min_{x\in D} e^{b_2(x)})^{-1}(\left\|e^{b_1}\right\|_{C(D)} + \left\|e^{b_2}\right\|_{C(D)})\,\|b_1 - b_2\|_{C(D)}\,\|f\|_{H^{-1}}\,.$$

According to [3, Proposition 2.3], all the random variables $\min_{x\in D} e^{b_i(x)})^{-1}$ and $\left\|e^{b_i}\right\|_{C(D)}$, $i = 1, 2$ have any moments of finite order. Then, we obtain the pathwise Lipschitz continuity of the operator G

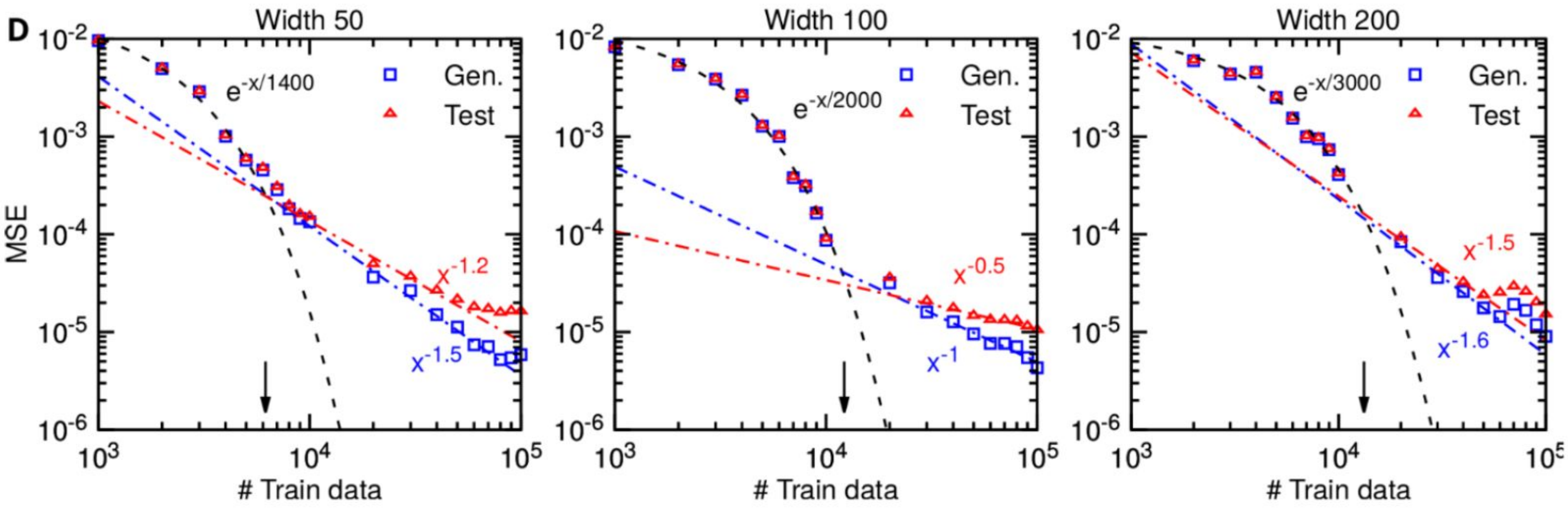
$$\|\mathcal{G}(b_1)(\omega) - \mathcal{G}(b_2)(\omega)\|_{H^1} \leq C(\omega)\,\|b_1 - b_2\|_{C(D)}\,.$$

Here $C(\omega) = (\min_{x\in D} e^{b_1(x)})^{-1}(\min_{x\in D} e^{b_2(x)})^{-1}(\left\|e^{b_1}\right\|_{C(D)} + \left\|e^{b_2}\right\|_{C(D)})\,\|f\|_{H^{-1}}$.

Lu L, Jin P, Pang G, Zhang Z, Karniadakis GE. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. Nature Machine Intelligence. 2021 Mar;3(3):218-29

Experiment Results: Gravity Pendulum

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



Test/generalization error:

- Small dataset: exponential convergence
- Large dataset: polynomial rates
- Smaller network has earlier transition point

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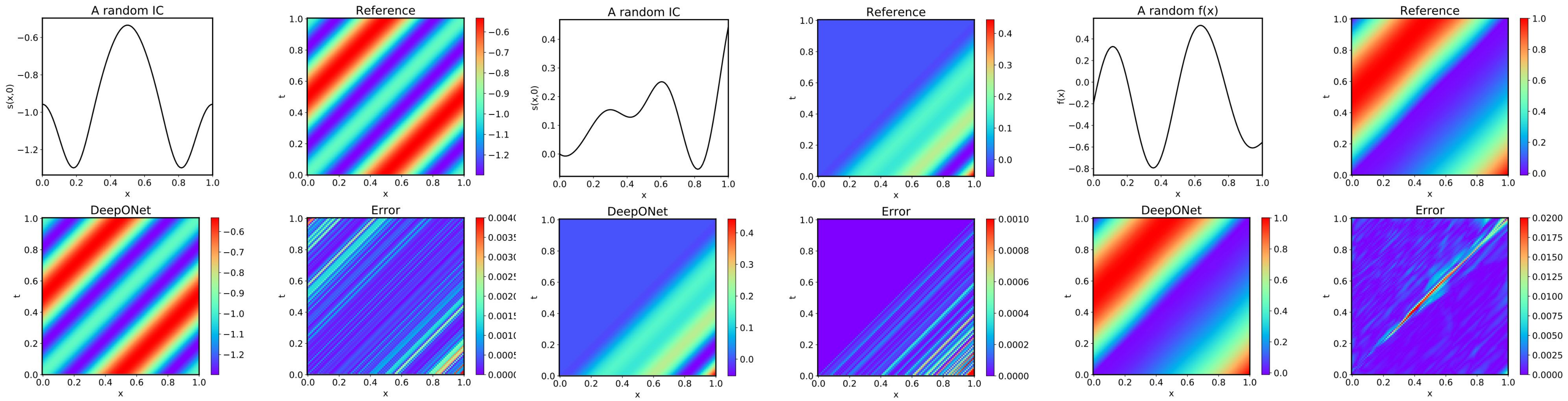
Experiment Results: Advection Equation

$$\frac{\partial s}{\partial t} + a(x)\frac{\partial s}{\partial x} = 0, \quad x \in [0,1], t \in [0,1]$$



Case	$a(x)$	IC $s(x,0)$	BC	Input	Length scale l	Test MSE
I	1	$f(\sin^2(\pi x))$	Periodic	$s(x,0)$	0.5	$1.8 \times 10^{-6} \pm 4.2 \times 10^{-7}$
II	1	$xf(x)$	$s(0,t)=0$	$s(x,0)$	0.2	$3.7 \times 10^{-7} \pm 1.8 \times 10^{-7}$
III	$1 + 0.1 \cdot f(x)$	x^2	$s(0,t)=\sin(\pi t)$	$f(x)$	0.2	$1.6 \times 10^{-5} \pm 6.8 \times 10^{-6}$
IV	$1 + 0.1 \cdot \frac{f(x)+f(1-x)}{2}$	$\sin(2\pi x)$	Periodic	$f(x)$	0.2	$3.2 \times 10^{-5} \pm 1.4 \times 10^{-5}$

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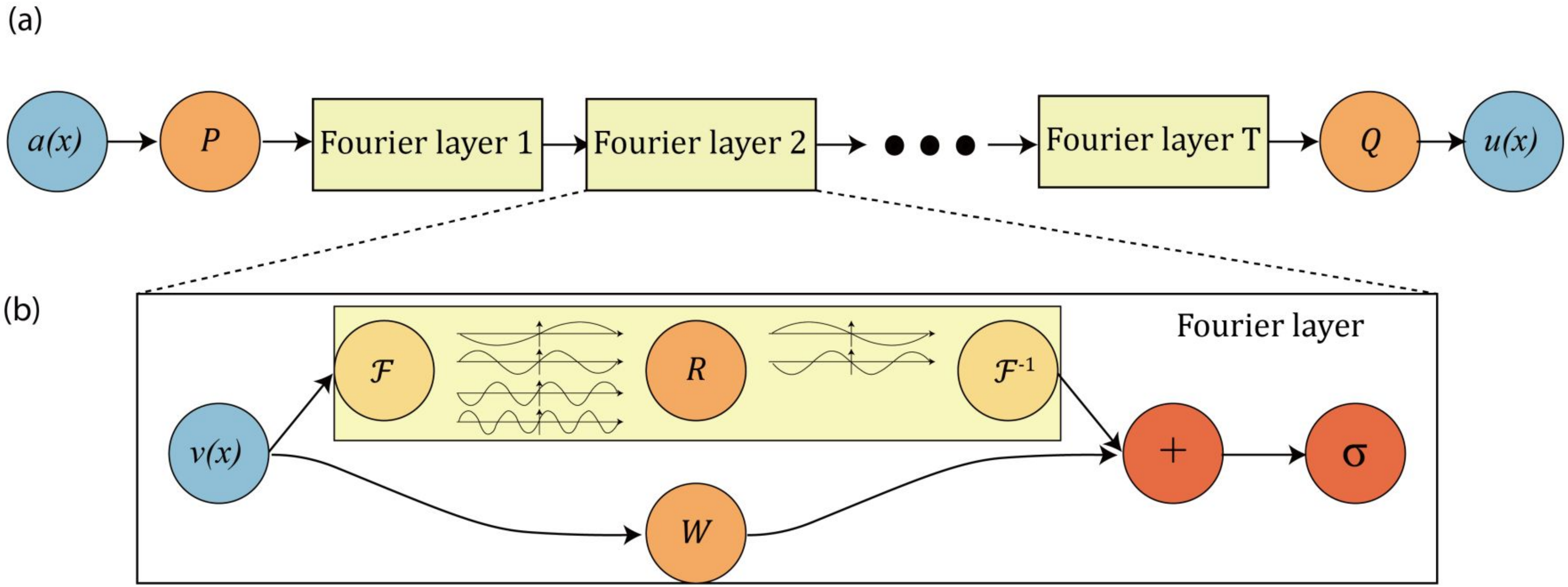
DeepONets for learning operator

- DeepONet
  - 16 ODEs/PDEs (nonlinear, fractional & stochastic) (*Lu et al., Nature Mach Intell, 2021*)
  - Bubble growth dynamics (*Lin, et al., J Chem Phys, 2021; Lin, et al., J Fluid Mech, 2021*)
  - Linear instability waves in high-speed boundary layers (*Di Leoni, et al., arXiv:2105.08697*)

- DeepM&Mnet
  - Electroconvection (*Cai, et al., J Comput Phys, 2021*)
  - Hypersonics (*Mao, et al., J Comput Phys, 2021*)

- Extensions of DeepONet, e.g., POD-DeepONet, MIO-Net, PI-DeepONet, V-DeepONet…

Fourier Neural Operator



Li Z, Kovachki N, Azizzadenesheli K, Liu B, Bhattacharya K, Stuart A, Anandkumar A. Fourier neural operator for parametric partial differential equations. arXiv preprint arXiv:2010.08895. 2020 Oct 18.

Structure of FNO

Step 1: Function value $v(x)$ is lifted to a higher dimensional representation $z_0(x)$ by

$$z_0(x) = P(v(x)) \in \mathbb{R}^{d_z}$$

Transformation $P : \mathbb{R} \to \mathbb{R}^{d_z}$ is a shallow fully-connected NN or simply a linear layer. d_z is like the channel size in CNN.

Step 2: L Fourier layers are applied iteratively to z_0. z_L is the output of the last Fourier layer, and the dimension of $z_L(x)$ is d_z.

Step 3: Transformation $Q : \mathbb{R}^{d_z} \to \mathbb{R}$ is applied to project $z_L(x)$ to the output by

$$u(x) = Q(z_L(x))$$

Q is parameterized by a fully-connected NN.

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Fourier Layer using FFT

For the output of the lth Fourier layer z_l with d_v channels:

Step 1: Compute the transform by FFT $\mathcal{F}$ and inverse FFT $\mathcal{F}^{-1}$:

$$\mathcal{F}^{-1}\left(R_l \cdot \mathcal{F}(z_l)\right)$$

$\mathcal{F}$ is applied to each channel of z_l separately Truncate the higher modes of $\mathcal{F}(z_l)$, keeping only the first k Fourier modes in each channel. So $\mathcal{F}(z_l)$ has the shape $d_v \times k$.

Step 2: Apply a different (complex-number) weight matrix of shape $d_v \times d_v$ for each mode index of $\mathcal{F}(z_l)$ Have k trainable matrices, which form a weight tensor $R_l \in \mathbb{C}^{d_v \times d_v \times k}$. $R_l \cdot \mathcal{F}(z_l)$ has the same shape of $d_v \times k$ as $\mathcal{F}(z_l)$.

Step 3: Inverse FFT Need to append zeros to $R_l \cdot \mathcal{F}(z_l)$ to fill in the truncated modes. Moreover, in each Fourier layer, a residual connection with a weight matrix $W_l \in \mathbb{R}^{d_v \times d_v}$. The output of the $(l+1)$th Fourier layer z_{l+1} is $\boldsymbol{z}_{l+1} = \sigma\left(\mathcal{F}^{-1}\left(R_l \cdot \mathcal{F}\left(\boldsymbol{z}_l\right)\right) + W_l \cdot \boldsymbol{z}_l + \boldsymbol{b}_l\right)$

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DeepONet and FNO

Then $u(x,t)$ is a rational function in $\mathbf{V}_m := (V_0, V_1, \cdots, V_{m-1})^\top$. By [Telgarsky 2017], there exists $\tilde{g}^{\mathcal{N}}(\mathbf{V}_m; \theta_{x,t})$ of size $O(m^2 \ln(\epsilon^{-1}))$ for fixed x, t s.t.

$$\sup_{u_0 \in S} \mid \tilde{g}^{\mathcal{N}}(\mathbf{V}_m; \theta_{x,t})\Big) - G(u_0) \mid \leq C\epsilon$$
$$S := \{v : \|v\|_{L^\infty} \leq M_0, \|\partial_x v\|_{L^\infty} \leq M_1\}$$

- $\tilde{g}^{\mathcal{N}}(\mathbf{V}_m; \theta_{x,t}))$ can be further approximated by a ReLU network
- $g^{\mathcal{N}}(\mathbf{u}_{0,m}; \Theta_{x,t})$ with input $\mathbf{u}_{0,m}$ (initial values).
- $g^{\mathcal{N}}(\mathbf{u}_{0,m}; \Theta_{x,t})$ can be viewed as FNO.
- $g^{\mathcal{N}}(\mathbf{u}_{0,m}; \Theta_{x,t})$ can serve as the branch of the DeepONet

$\sum_{k=1}^{p} g^{\mathcal{N}}(\mathbf{u}_{0,m}; \Theta_{x_k,t}) L_k$, where x_k 's are Fourier collocation points and $L_k(x)'s$ are the Lagrange basis.

Conclusion

- Take $\epsilon = m^{-1}$ (accuracy), the size of FNO is $O(m^3 \ln(m))$ while the size of DeepONet is $O(m^3 \ln(m))$ (branch) $+O(m)$ (trunk).
- In general, we connect FNO $F^{\mathcal{N}}(v)$ and DeepONet by

$$G^v(v)(x) = \sum_{k=1}^{m} F^N(v)(x_k) L_k(x)$$

Consider the Burgers' equation $u_t + uu_x = \kappa u_{xx}$ with periodic boundary condition $u(x-\pi, t) = u(x+\pi, t), x \in R$. Then, by the Cole-Hopf transformation,

$$\begin{aligned} u(x,t) =: G(u_0) &= \frac{-2\kappa \cdot \int_{\mathbb{R}} \partial_x \mathcal{K}(x,y,t) v_0(y) dy}{\int_{\mathbb{R}} \mathcal{K}(x,y,t) v_0(y) dy} \\ &\approx \frac{-2\kappa \int_{\mathbb{R}} \mathcal{K}(x,y,t) v_0(y) dy}{\int_{\mathbb{R}} \mathcal{K}(x,y,t) (\mathcal{I}_m v_0)(y) dy} \\ &= \frac{V_0 c_0^1 + V_1 c_1^1 + \cdots + V_{m-1} c_{m-1}^1}{V_0 c_0^2 + V_1 c_1^2 + \cdots + V_{m-1} c_{m-1}^2} \end{aligned}$$

where $\mathcal{K}$ is the heat kernel, $\mathcal{I}_m$ is the Fourier interpolation operator and

$$V_0 = 1, V_j = \exp\left(-\sum_k \int_0^{x_j} L_k(y) dy \frac{u_0(y_k)}{2\kappa}\right), j = 1, \cdots, m-1$$

$$c_j^1(x,t) = -2\kappa_i \int_0^x \left(\sum_l \partial_x \mathcal{K}(x, y + 2\pi l, t)\right) L_j(y) dy$$

$$c_j^2(x,t) = \int_0^x \left(\sum_j \mathcal{K}(x, y + 2\pi l, t)\right) L_j(y) dy$$

Conclusion

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Applications of Neural Operators

DeepONet for Approximating Functionals: Predicting unsteady pressure and lift/drag-force coefficients

- Simulation of NACA0012 airfoil (Nektar by Z. Wang)

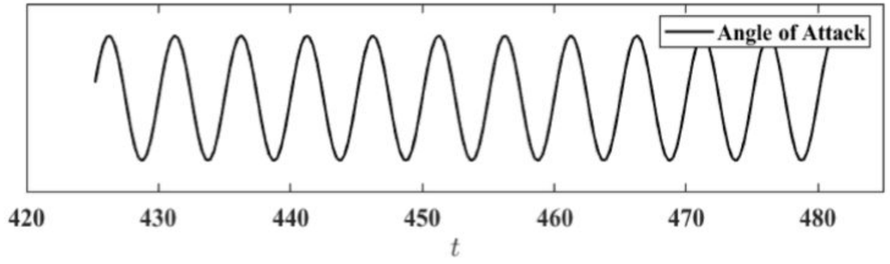
inflow

$$u = U_\infty \cos\left(\frac{\alpha_0 \pi}{180} \times \frac{\sin(2f\pi t) + 1.0}{2}\right),$$

$$v = U_\infty \sin\left(\frac{\alpha_0 \pi}{180} \times \frac{\sin(2f\pi t) + 1.0}{2}\right),$$

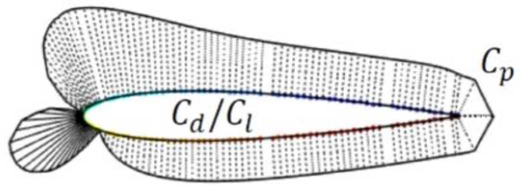
$$\alpha = 15^o \quad f = 0.2 \quad U_\infty = 1 \quad Re = 2500$$

- Generate time-dependent AOA



predict

- Time-dependent coefficients of drag, lift, pressure



Applications of Neural Operators

DeepONet for Approximating Functionals: Predicting unsteady pressure and lift/drag-force coefficients

- Simulation of NACA0012 airfoil (Nektar by Z. Wang)

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$\alpha = 15^o$
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$U_\infty = 1$
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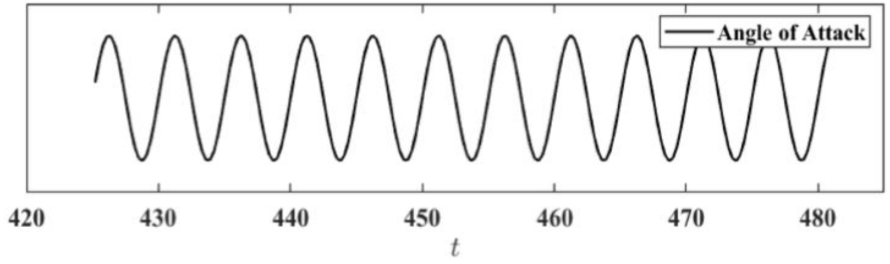
- Generate time-dependent AOA



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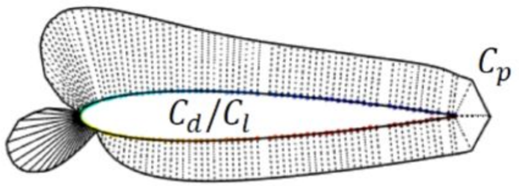
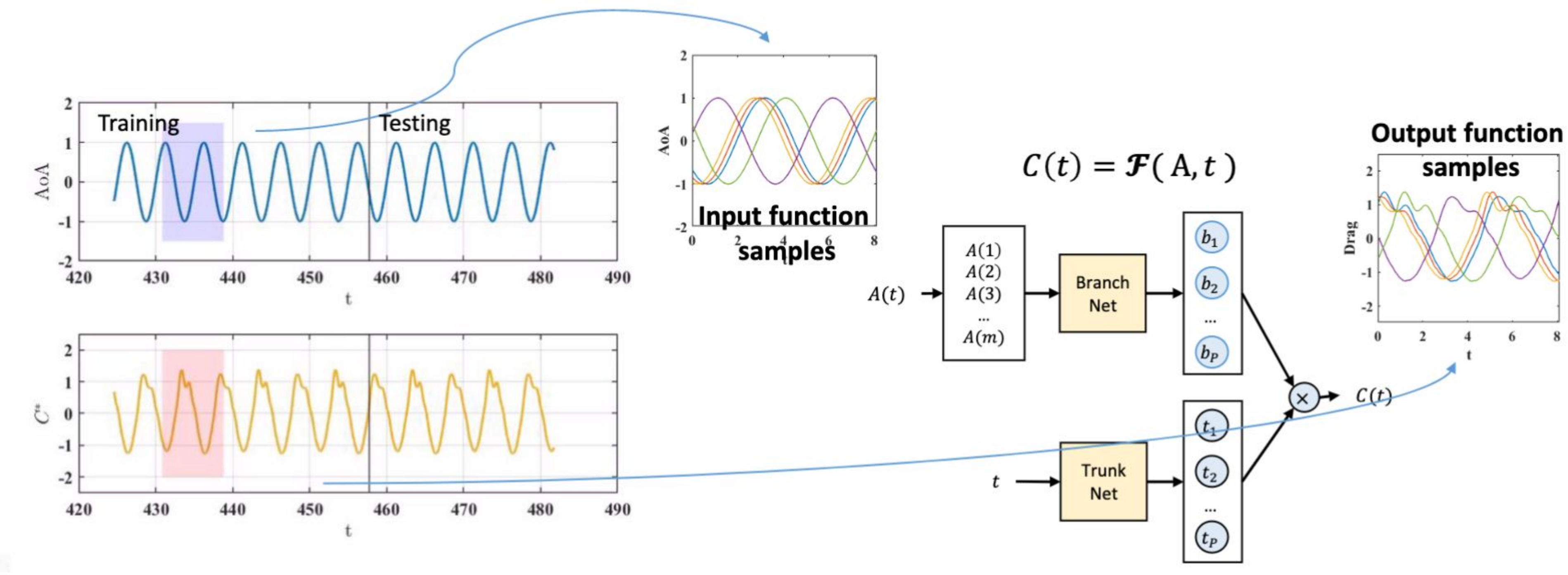


Applications of Neural Operators

DeepONet for Approximating Functionals: Predicting unsteady pressure and lift/drag-force coefficients

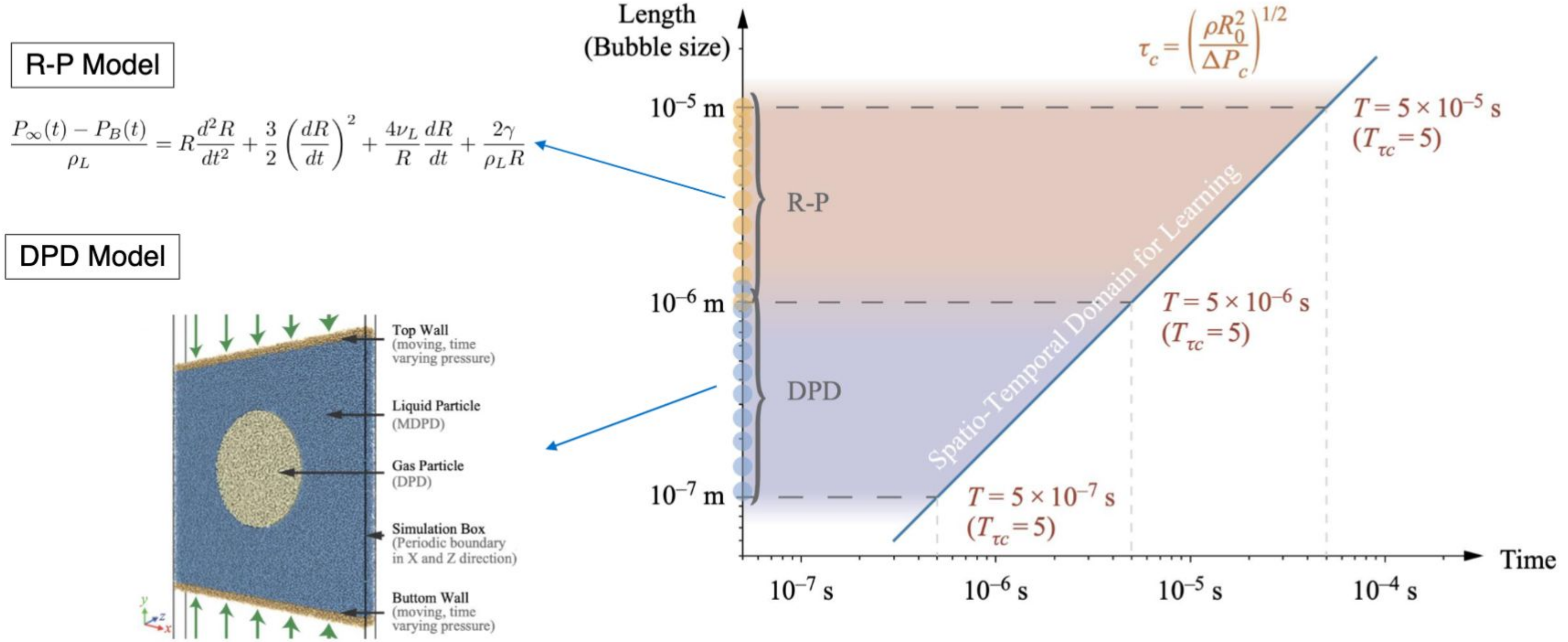
- Predicting drag/lift coefficient
- Cut the time-dependent signal into pieces, to generate a bunch of input-output pairs



Applications of Neural Operators

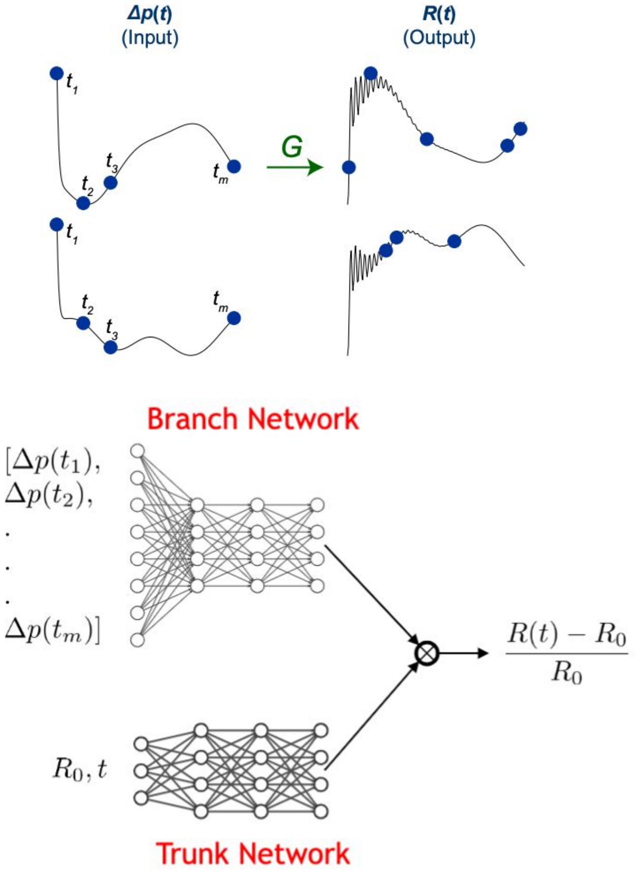
DeepONet for Bubble Dynamics

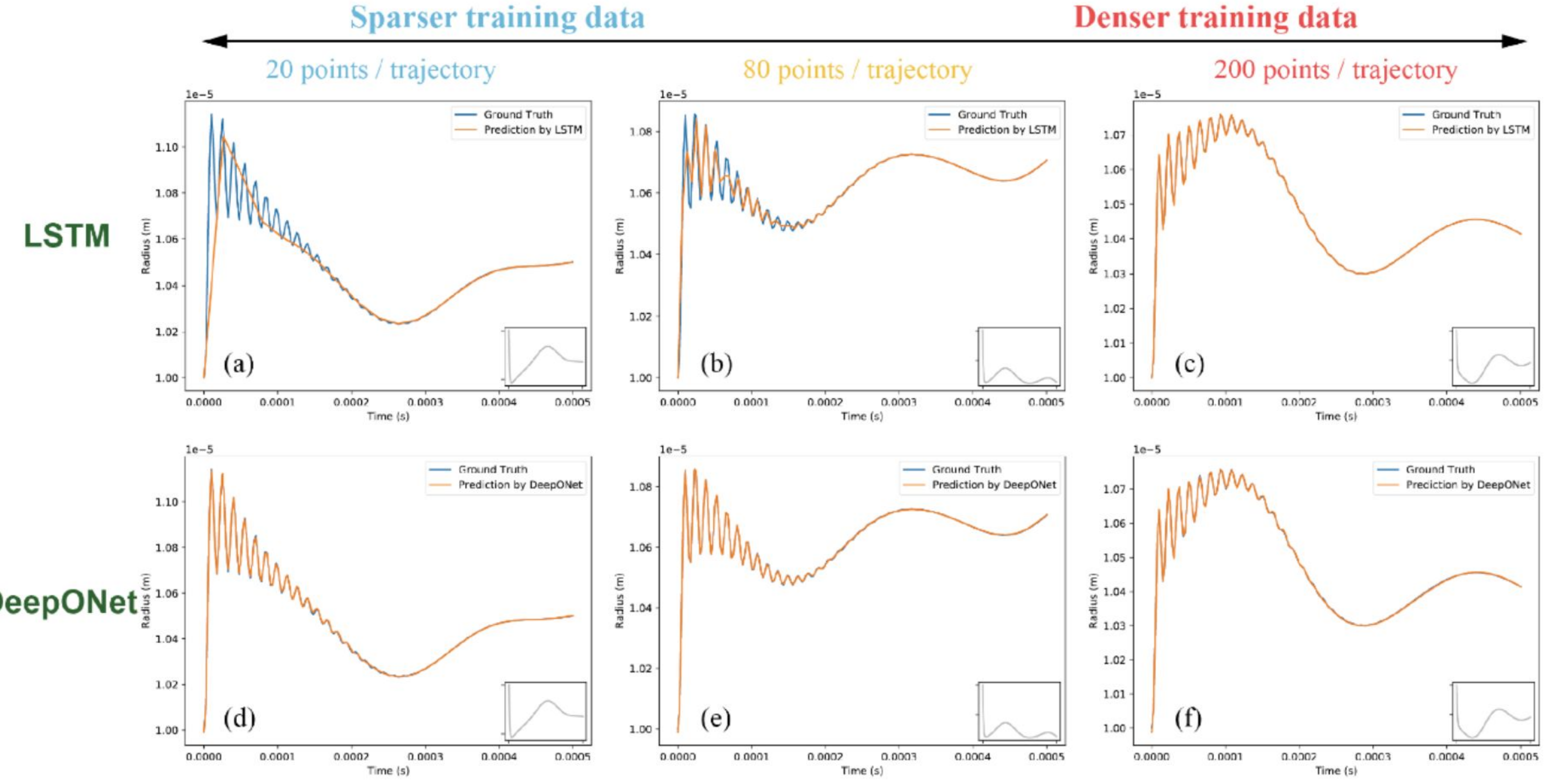
- Rayleigh-Plesset equation is an ordinary differential equation which governs the dynamics of a spherical bubble in an infinite body of imcomporessible fluid
- For nanobubbles, the thermal fluctuation cannot be ignored, and trainning data are generated by particle simulation



Applications of Neural Operators

DeepONet for Bubble Dynamics





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THANK YOU