Ensemble and Mixture-of-Experts DeepONets for Operator Learning

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The Oden Institute for Computational Engineering and Sciences

The University of Texas at Austin

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- The approximation $\hat{\mathcal{G}} : \mathcal{U} \times \Theta \to \mathcal{V}$, where the parameters Θ are picked to minimize $\|\mathcal{G} - \hat{\mathcal{G}}\|$.

Operator Learning

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- Laplacian: $u(x, y) \rightarrow \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$
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Deep Operator Network (DeepONet)

- DeepONets consist of two neural networks[1],
  - **Branch**: Nonlinear encoding of the input functions; $\boldsymbol{\beta} : \mathbb{R}^{N_x} \rightarrow \mathbb{R}^p$.
  - **Trunk**: Nonlinear basis for the output functions; $\boldsymbol{\tau} : \mathbb{R}^{d_v} \rightarrow \mathbb{R}^p$.

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- The DeepONet can be seen as an p-dimensional inner product between the branch and the trunk:

$$\hat{\mathcal{G}}(u)(y) = \langle \boldsymbol{\tau}(y), \boldsymbol{\beta}(u) \rangle + b_0, \tag{1}$$

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- $\|v_i(y) - \hat{\mathcal{G}}(u_i)(y)\|_2^2$ is minimized over N training function pairs.

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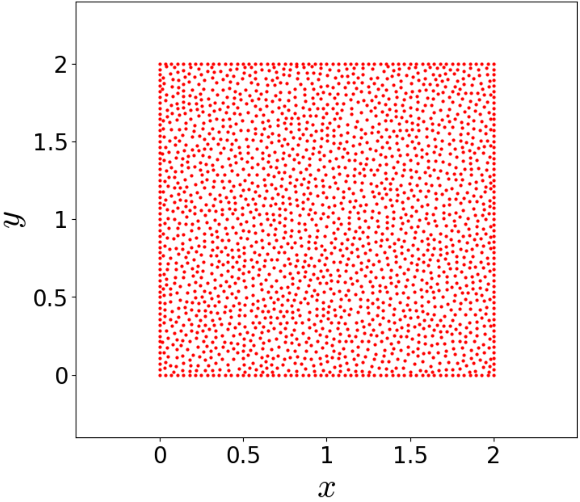
- We partition the output function domain Ω into P overlapping spherical patches that form a cover of Ω; Ω_k, $k = 1, \ldots, P$.



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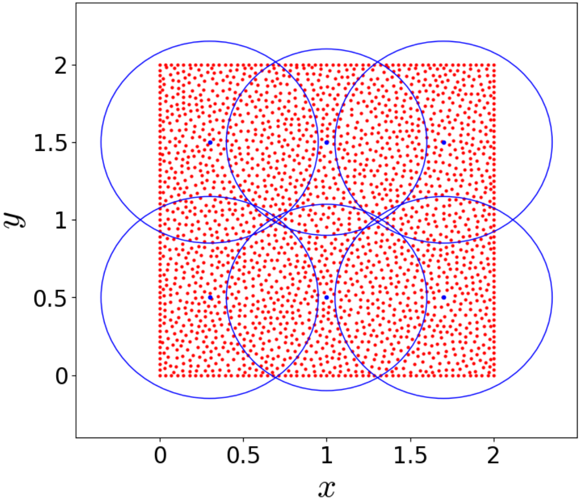

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- Then, *blend* them together to produce one global trunk.
- The PoU-MoE trunk is written as,

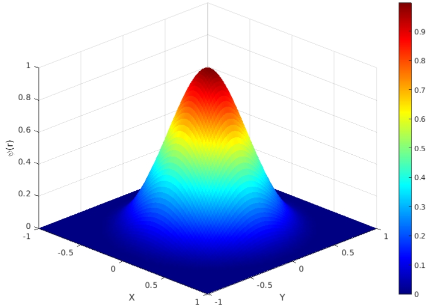
$$\boldsymbol{\tau}_{\text{PU}}(y) = \sum_{k=1}^{P} w_k(y)\boldsymbol{\tau}_k(y), \tag{2}$$

where the weights functions w_k are chosen to be the compactly supported $\mathbb{C}^2\left(\mathbb{R}^3\right)$ Wendland kernel.

Partition-of-Unity Mixture-of-Experts (PoU-MoE) Trunk

- The scaled and shifted Wendland kernel on patch Ω_k is given by,

$$\psi_k(y, y^c) = \psi_k\left(\frac{\|y - y_k^c\|}{\rho}\right) = \psi_k(r) = (1 - r)_+^4(4r + 1). \tag{3}$$



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- The weight functions are given by,

$$w_k(y) = \frac{\psi_k(y)}{\sum_j \psi_j(y)}, \; k, j = 1, \ldots, P, \tag{5}$$

- Satisfy $\sum_k w_k(y) = 1$.

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  - Is sparse in its experts $\boldsymbol{\tau}_k$.
  - Constitutes a global set of basis functions.
  - Is a universal approximator.

Proper Orthogonal Decomposition (POD) Trunk

- The POD trunk [2] uses the output functions' eigenvectors corresponding to the p smallest eigenvalues as a set of **global** basis functions.

$$\boldsymbol{\tau}_{\text{POD}}(y) = \begin{bmatrix} \phi_1(y) & \phi_2(y) & \dots & \phi_p(y) \end{bmatrix}, \tag{6}$$

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- In this work, we use a **"Modified-POD"** trunk that includes the mean function ϕ_0 in the set of basis functions.

$$\boldsymbol{\tau}_{\text{Modified-POD}}(y) = \begin{bmatrix} \phi_0(y) & \phi_1(y) & \dots & \phi_{p-1}(y) \end{bmatrix}, \tag{7}$$

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$$\hat{\mathcal{G}}(u, y) = \left\langle \underbrace{[\boldsymbol{\tau}_1(y), \boldsymbol{\tau}_2(y), \boldsymbol{\tau}_3(y)]}_{\text{Ensemble trunk}}, \hat{\boldsymbol{\beta}}(u) \right\rangle + b_0, \tag{8}$$

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where

$\boldsymbol{\tau}_1 : \mathbb{R}^{d_v} \to \mathbb{R}^{p_1}, \boldsymbol{\tau}_2 : \mathbb{R}^{d_v} \to \mathbb{R}^{p_2}, \boldsymbol{\tau}_3 : \mathbb{R}^{d_v} \to \mathbb{R}^{p_3}$

$\boldsymbol{\beta} : \mathbb{R}^{N_x} \to \mathbb{R}^{p_1+p_2+p_3}$

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- The ensemble trunk is also a universal approximator.

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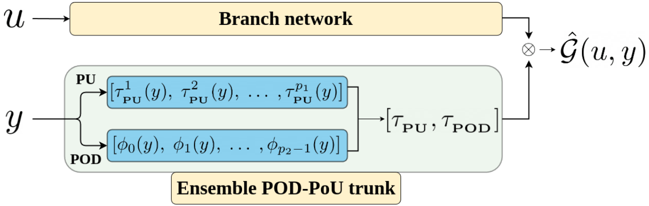
- **Vanilla-POD-PoU**: Adding a vanilla trunk (extra trainable parameters) to a POD-PoU ensemble.
- $(P + 1)$**-Vanilla**: Simple overparametrization. We use $P + 1$ vanilla trunks in this model, where P is the number of PoU-MoE patches.

POD-PoU Ensemble



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2D Darcy Flow

$$-\nabla \cdot (K(y)\,\nabla u(y)) = f(y), \;\; y \in \Omega, \tag{9}$$

$$u(y) \sim \mathcal{GP}\left(0, \mathcal{K}(y_1, y_1')\right), \tag{10}$$

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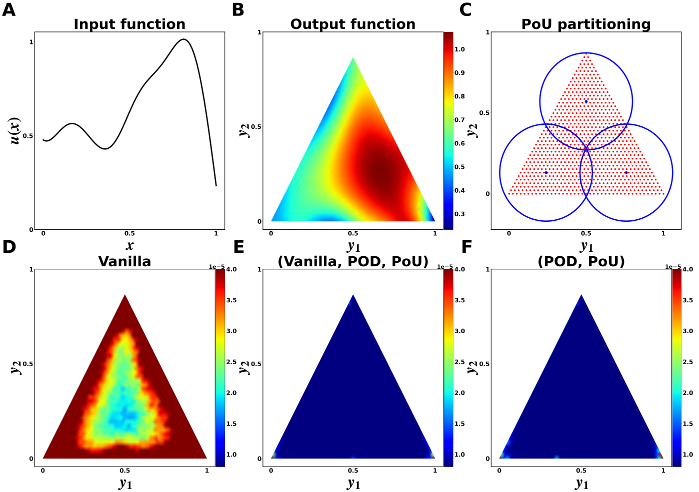
- $K(y)$ is the permeability field.
- Ω was a triangular domain.
- **Goal:** learn the solution operator $\mathcal{G} : u(y)|_{\partial\Omega} \to u(y)|_{\Omega}$.

2D Darcy Flow



	Vanilla	Vanilla-POD-PoU	(POD, PoU)
Relative l_2 error	0.857 ± 0.08	$\mathbf{0.187 \pm 0.02}$	0.204 ± 0.02

2D Lid-driven Cavity Flow

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla \mathbf{p} + \nu \Delta \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0, \;\; y \in \Omega, \;\; t \in T, \tag{11}$$

$$\mathbf{u} = \mathbf{u}_b, \tag{12}$$

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- $\Omega = [0, 1]^2$.
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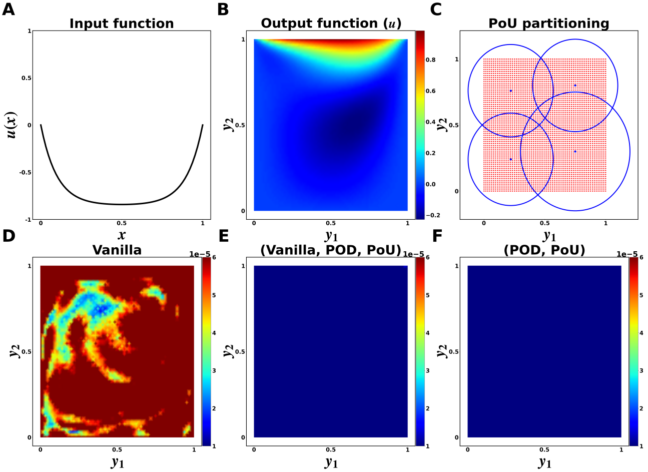

	Vanilla	Vanilla-POD-PoU	(POD, PoU)
Relative l_2 error	5.53 ± 1.05	0.229 ± 0.01	$\mathbf{0.204 \pm 0.01}$

2D Reaction-Diffusion

$$\frac{\partial c}{\partial t} = k_{\text{on}} \left(R - c\right) c_{\text{amb}} - k_{\text{off}}\ c + \nu \Delta c,\ \ y \in \Omega,\ \ t \in T, \tag{13}$$

$$\nu \frac{\partial c}{\partial n} = 0,\ \ y \in \partial\Omega, \tag{14}$$

$$c(y, 0) \sim \mathcal{U}(0, 1). \tag{15}$$

- k_{on} and k_{off} are constants, and $c_{\text{amb}}(y, t)$ is a background source of the chemical.

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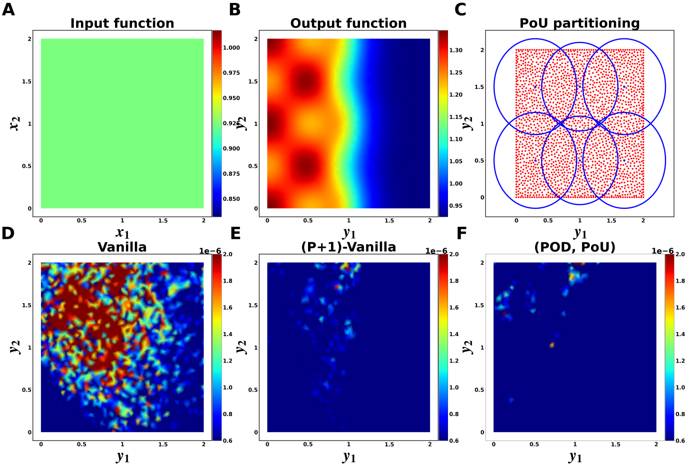
- k_{on} and k_{off} are constants, and $c_{\text{amb}}(y,t)$ is a background source of the chemical.
- $\Omega = [0,2]^2$ and $T = [0, 0.5]$.
- We choose k_{on} and k_{off} to introduce a sharp spatial discontinuity in the solution at $y_1 = 1$.

$$k_{\text{on}} = \begin{cases} 2, & y_1 \leq 1.0, \\ 0, & \text{otherwise} \end{cases}, \quad k_{\text{off}} = \begin{cases} 0.2, & y_1 \leq 1.0, \\ 0, & \text{otherwise} \end{cases}, \tag{16}$$

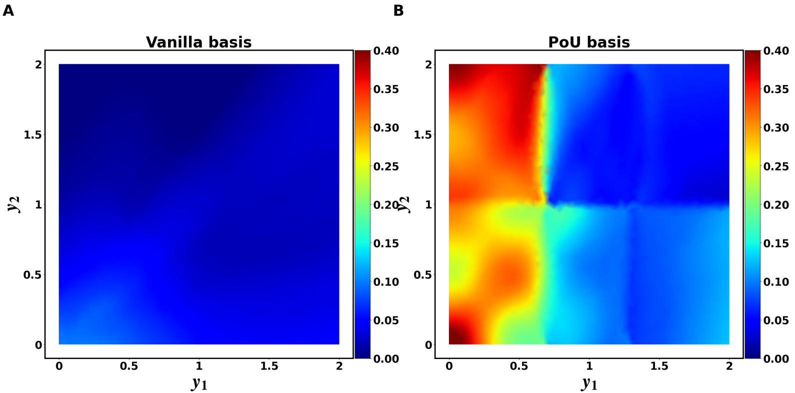
- **Goal:** learn the solution operator $\mathcal{G} : c(y,0) \to c(y,0.5)$.

2D Reaction-Diffusion



	Vanilla	$(P+1)$-Vanilla	(POD, PoU)
Relative l_2 error	0.144 ± 0.01	0.0644 ± 0.02	$\mathbf{0.0539 \pm 4e-5}$

Spatial Locality



- Basis functions corresponding to the largest branch coefficients, i.e., the most "important" basis functions.
- The PoU basis spatially varies significantly more than the vanilla basis.
- The PoU-MoE trunk learns spatially local features, which improves accuracy.

3D Variable-Coefficient Reaction-Diffusion

$$\frac{\partial c}{\partial t} = k_{\text{on}}\left(R - c\right) c_{\text{amb}} - k_{\text{off}}\ c + \nabla \cdot \left(K(y)\nabla c\right),\ \ y \in \Omega,\ \ t \in T, \tag{17}$$

$$K(y)\frac{\partial c}{\partial n} = 0, y \in \partial\Omega, \tag{18}$$

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- Sharp point of discontinuity at $y_1 = 0$.

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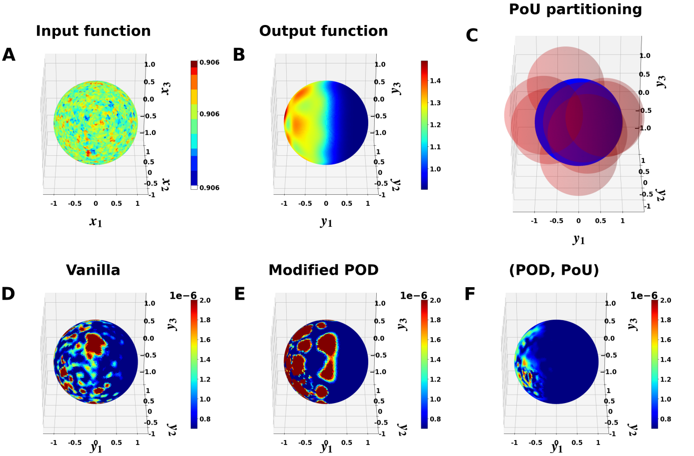
- Ω was the unit ball, and $T = [0, 0.5]$.
- Sharp point of discontinuity at $y_1 = 0$.
- $K(y)$ was chosen to introduce steep gradients in the diffusion term, defined as.

$$K(y) = B + \frac{C}{\tanh(A)}\left((A-3)\tanh(8y_1 - 5) - (A - 15)\tanh(8y_1 + 5) + A\tanh(A)\right), \tag{20}$$

  where $A = 9$, $B = 0.0215$, and $C = 0.005$.
- **Goal:** learn the solution operator $\mathcal{G} : c(y, 0) \to c(y, 0.5)$.

3D Variable-Coefficient Reaction-Diffusion



	Vanilla	Modified-POD	(POD, PoU)
Relative l_2 error	0.127 ± 0.03	$0.155 \pm 4e-5$	$\mathbf{0.0576 \pm 0.05}$

Insights

Trunk Choices	Darcy flow	Cavity flow	2D RD	3D RD
POD global modes	Yes	No	No	No
modified POD global modes	Yes	No	No	No
Adding POD global modes	Yes	Yes	Yes	No
Adding spatial locality	No	Yes	Yes	No
Only POD global modes + spatial locality	Yes	**Yes**	**Yes**	**Yes**
Only POD global modes + spatial locality + vanilla trunk	**Yes**	Yes	Yes	No
Adding excessive overparametrization	No	Yes	Yes	No

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- Yes/no refers to whether the strategy beats a vanilla-DeepONet, bold refers to the best accuracy.
- Answers the question, "What makes a good ensemble trunk?"

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- Simple overparametrization ($(P+1)$-Vanilla DeepONet) is not enough and sometimes deteriorates accuracy; **a judicial combination of localized and global basis functions is vital**.
- The novel PoU-MoE trunk captures spatially local features.

Conclusion

- The ensemble DeepONet, a method of enriching the basis functions of the DeepONet.
- The POD-PoU ensemble consistently beats the vanilla-DeepONet across all problems (**2-4x accuracy improvement**).
- Simple overparametrization (($P + 1$)-Vanilla DeepONet) is not enough and sometimes deteriorates accuracy; **a judicial combination of localized and global basis functions is vital**.
- The novel PoU-MoE trunk captures spatially local features.
- The PoU-MoE trunk brings expressivity in problems with steep gradients in either the input or output functions.

Future work

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- Extend PoU-MoE to adaptive partitioning strategies (trainable patch centers and patch radii, trainable patch shape).

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- Extend PoU-MoE to adaptive partitioning strategies (trainable patch centers and patch radii, trainable patch shape).
- Ensemble learning for other neural operators (FNO, GNO, etc.).

Thank you

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Error calculations

- For all experiments, we first computed the relative l_2 error for each test function, $e_{\ell_2} = \frac{\|\underline{\tilde{u}} - \underline{u}\|_2}{\|\underline{u}\|_2}$ where $\underline{u}$ was the true solution vector and $\underline{\tilde{u}}$ was the DeepONet prediction vector; we then computed the mean over those relative ℓ_2 errors.
- We also report a squared error (MSE) between the DeepONet prediction and the true solution averaged over N *functions* $e_{\mathrm{mse}}(y) = \frac{1}{N}\left(\tilde{u}(y) - u(y)\right)^2$.

Other results

Relative l_2 errors (as percentage) on the test dataset for the 2D **Darcy flow**, **cavity flow**, and **reaction-diffusion** problems, and the 3D **reaction-diffusion** problem. RD stands for reaction-diffusion.

	Darcy flow	Cavity flow	2D RD	3D RD
Vanilla	0.857 ± 0.08	5.53 ± 1.05	0.144 ± 0.01	0.127 ± 0.03
POD	0.297 ± 0.01	$7.94 \pm 2e-5$	$5.06 \pm 8e-7$	9.40 ± 8
Modified-POD	0.300 ± 0.04	$7.93 \pm 2e-5$	$0.131 \pm 4e-5$	$0.155 \pm 4e-5$
(Vanilla, POD)	0.227 ± 0.03	0.310 ± 0.03	$0.0751 \pm 4e-5$	5.24 ± 10.4
$(P+1)$-Vanilla	1.19 ± 0.06	2.17 ± 0.3	0.0644 ± 0.02	5.25 ± 10.3
(Vanilla, PoU)	0.976 ± 0.03	1.06 ± 0.05	0.0946 ± 0.03	5.25 ± 10.3
(POD, PoU)	0.204 ± 0.02	$\mathbf{0.204 \pm 0.01}$	$\mathbf{0.0539 \pm 4e-5}$	$\mathbf{0.0576 \pm 0.05}$
(Vanilla, POD, PoU)	$\mathbf{0.187 \pm 0.02}$	0.229 ± 0.01	$0.0666 \pm 8e-5$	5.22 ± 10.4

Runtime results

Table: Average time per training epoch in seconds. RD stands for reaction-diffusion.

	Darcy flow	Cavity flow	2D RD	3D RD
Vanilla	$8.93e-4$	$3.99e-4$	$2.97e-4$	$2.10e-4$
POD	$5.19e-4$	$2.46e-4$	$2.06e-4$	$1.22e-4$
Modified-POD	$6.86e-4$	$2.49e-4$	$2.08e-4$	$1.22e-4$
(Vanilla, POD)	$9.80e-4$	$3.92e-4$	$3.03e-4$	$2.32e-4$
$(P+1)$-Vanilla	$1.10e-3$	$8.51e-4$	$7.27e-4$	$9.45e-4$
Vanilla-PoU	$8.67e-4$	$9.52e-4$	$1.03e-3$	$1.39e-3$
POD-PoU	$6.74e-4$	$8.21e-4$	$9.24e-4$	$1.28e-3$
Vanilla-POD-PoU	$8.55e-4$	$9.48e-4$	$1.05e-3$	$1.43e-3$

Runtime results

Table: Inference time on the test dataset in seconds. RD stands for reaction-diffusion.

	Darcy flow	Cavity flow	2D RD	3D RD
Vanilla	$1.66e-4$	$1.39e-4$	$1.32e-4$	$7.20e-5$
POD	$1.57e-4$	$1.12e-4$	$1.12e-4$	$6.42e-5$
Modified-POD	$1.34e-4$	$1.08e-4$	$9.94e-5$	$6.62e-5$
(Vanilla, POD)	$1.69e-4$	$1.33e-4$	$1.20e-4$	$7.76e-5$
$(P+1)$-Vanilla	$2.08e-4$	$2.12e-4$	$1.71e-4$	$1.48e-4$
Vanilla-PoU	$1.91e-4$	$2.42e-4$	$2.21e-4$	$2.37e-4$
POD-PoU	$1.63e-4$	$1.94e-4$	$1.96e-4$	$2.30e-4$
Vanilla-POD-PoU	$2.00e-4$	$2.18e-4$	$2.28e-4$	$2.41e-4$

Universal Approximation Theorem - PoU-MoE Trunk

Theorem

Let $\mathcal{G} : \mathcal{U} \to \mathcal{V}$ be a continuous operator. Define $\mathcal{G}^\dagger$ as $\mathcal{G}^\dagger(u)(y) = \left\langle \boldsymbol{\beta}(u; \theta_b), \sum_{j=1}^{P} w_j(y)\boldsymbol{\tau}_j(y; \theta_{\boldsymbol{\tau}_j}) \right\rangle + b_0$, where $\boldsymbol{\beta} : \mathbb{R}^{N_x} \times \Theta_{\boldsymbol{\beta}} \to \mathbb{R}^p$ is a branch network embedding the input function u, $\boldsymbol{\tau}_j : \mathbb{R}^{d_v} \times \Theta_{\boldsymbol{\tau}_j} \to \mathbb{R}^p$ are trunk networks, b_0 is a bias, and $w_j : \mathbb{R}^{d_v} \to \mathbb{R}$ are compactly-supported, positive-definite weight functions that satisfy the partition of unity condition $\sum_j w_j(y) = 1, j = 1, \ldots, P$. Then $\mathcal{G}^\dagger$ can approximate $\mathcal{G}$ globally to any desired accuracy, i.e.,

$$\mathcal{G}(u)(y) - \mathcal{G}^\dagger(u)(y)\|_{\mathcal{V}} \leq \epsilon, \tag{21}$$

where $\epsilon > 0$ can be made arbitrarily small.

Universal Approximation Theorem - PoU-MoE Trunk

Proof

$$\begin{aligned}
\|\mathcal{G}(u)(y) - \mathcal{G}^\dagger(u)(y)\|_{\mathcal{V}} &= \left\| \mathcal{G}(u)(y) - \left\langle \boldsymbol{\beta}(u;\theta_b), \sum_{j=1}^{P} w_j(y)\boldsymbol{\tau}_j(y;\theta_{\boldsymbol{\tau}_j}) \right\rangle - b_0 \right\|_{\mathcal{V}}, \\
&= \left\| \underbrace{\left(\sum_{j=1}^{P} w_j(y)\right)}_{=1} \mathcal{G}(u)(y) - \left\langle \boldsymbol{\beta}(u;\theta_b), \sum_{j=1}^{P} w_j(y)\boldsymbol{\tau}_j(y;\theta_{\boldsymbol{\tau}_j}) \right\rangle \right. \\
&\qquad \left. - \underbrace{\left(\sum_{j=1}^{P} w_j(y)\right)}_{=1} b_0 \right\|_{\mathcal{V}}, \\
&= \left\| \sum_{j=1}^{P} w_j(y) \left(G(u)(y) - \left\langle \boldsymbol{\beta}(u;\theta_b), \boldsymbol{\tau}_j(y;\theta_{\boldsymbol{\tau}_j}) \right\rangle - b_0 \right) \right\|_{\mathcal{V}}, \\
&\leq \sum_{j=1}^{P} w_j(y) \|\mathcal{G}(u)(y) - \left\langle \boldsymbol{\beta}(u;\theta_b), \boldsymbol{\tau}_j(y;\theta_{\boldsymbol{\tau}_j}) \right\rangle - b_0\|_{\mathcal{V}}.
\end{aligned}$$

Universal Approximation Theorem - PoU-MoE Trunk

Given a branch network $\boldsymbol{\beta}$ that can approximate functionals to arbitrary accuracy, the (generalized) universal approximation theorem for operators automatically implies that a trunk network $\boldsymbol{\tau}_j$ (given sufficient capacity and proper training) can approximate the restriction of $\mathcal{G}$ to the support of $w_i(\mathbf{y})$ such that:

$$\|\mathcal{G}(u)(y) - \left\langle \boldsymbol{\beta}(u;\theta_b), \boldsymbol{\tau}_j(y;\theta_{\boldsymbol{\tau}_j}) \right\rangle - b_0\|_{\mathcal{V}} \leq \epsilon_j,$$

for all y in the support of w_j and any $\epsilon_j > 0$. Setting $\epsilon_j = \epsilon$, $j = 1, \ldots, P$, we obtain:

$$\|\mathcal{G}(u)(y) - \mathcal{G}^\dagger(u)(y)\|_{\mathcal{V}} \leq \epsilon \underbrace{\sum_{j=1}^{P} w_i(y)}_{=1},$$

$$\implies \|\mathcal{G}(u)(y) - \mathcal{G}^\dagger(u)(y)\|_{\mathcal{V}} \leq \epsilon.$$

where $\epsilon > 0$ can be made arbitrarily small. This completes the proof.

Universal Approximation Theorem - Ensemble Trunk

Theorem

Let $\mathcal{G} : \mathcal{U} \to \mathcal{V}$ be a continuous operator. Define $\hat{\mathcal{G}}$ as $\hat{\mathcal{G}}(u, y) = \left\langle \hat{\boldsymbol{\tau}}(y; \theta_{\boldsymbol{\tau}_1}; \theta_{\boldsymbol{\tau}_2}; \theta_{\boldsymbol{\tau}_3}), \hat{\boldsymbol{\beta}}(u; \theta_b) \right\rangle + b_0$, where $\hat{\boldsymbol{\beta}} : \mathbb{R}^{N_x} \times \Theta_{\hat{\boldsymbol{\beta}}} \to \mathbb{R}^{p_1+p_2+p_3}$ is a branch network embedding the input function u, b_0 is the bias, and $\hat{\boldsymbol{\tau}} : \mathbb{R}^{d_v} \times \Theta_{\hat{\boldsymbol{\tau}}_1} \times \Theta_{\hat{\boldsymbol{\tau}}_2} \times \Theta_{\hat{\boldsymbol{\tau}}_3} \to \mathbb{R}^{p_1+p_2+p_3}$ is an ensemble trunk network. Then $\hat{\mathcal{G}}$ can approximate $\mathcal{G}$ globally to any desired accuracy, i.e.,

$$\|\mathcal{G}(u)(y) - \hat{\mathcal{G}}(u)(y)\|_{\mathcal{V}} \leq \epsilon, \tag{22}$$

where $\epsilon > 0$ can be made arbitrarily small.

Proof.

This follows from the (generalized) universal approximation theorem[a] which holds for arbitrary branches and trunks. □

[a] Lu, Jin, et al. 2021.

Ensemble FNO

- FNOs consist of a *lifting* operator, a *projection* operator, and intermediate Fourier layers consisting of kernel-based integral operators.
- f_t denotes the intermediate function at the t^{th} Fourier layer. Then, f_{t+1} is given by

$$f_{t+1}(y) = \sigma\left(\int_{\Omega} \mathcal{K}(x,y)\, f_t(x)\, dx \;+\; W\, f_t(y)\right),\;\; x \in \Omega, \tag{23}$$

where σ is an activation function, $\mathcal{K}$ is a matrix-valued kernel, and W is the pointwise convolution.

- This is a projection of $f_t(x)$ onto a set of *global* Fourier modes.
- Incorporating a set of localized basis functions in an ensemble FNO using the PoU-MoE formulation:

$$f_{t+1}(y) = \sigma\left(\underbrace{\int_{\Omega} \mathcal{K}(x,y) f_t(x)\, dx}_{\text{Global basis}} + \underbrace{\sum_{k=1}^{P} w_k(y) \int_{\Omega_k} \mathcal{K}(x,y)\, f_t(x)|_{\Omega_k}\, dx}_{\text{Localized basis}} + W f_t(y)\right), \tag{24}$$

- The PoU-MoE formulation now combines a set of *localized* integrals, each of which is a projection of f_t onto a local Fourier basis.