

# Transfer and Multi-Task Learning in Physics-Based Applications with Deep Neural Operators

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# Can Neural Networks Predict in Real-Time (Autonomy)?



Courtesy: MIT, Michael Triantafyllou



### Can we predict the rupture of aneurysm?





### Can we predict the rupture of aneurysm?



Courtesy: Boston Children's Hospital, J. Marsden



### Data + Laws of Physics

The 5D Law: Dinky, Dirty, Dynamic, Deceptive Data

Three scenarios of Physics-Informed Learning Machines





### **Motivation**

$$k\left(\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2}\right) = f(x,y) \qquad \Omega = [0,1] \times [0,1]$$



**To Generalize:** Need an approach to learn to predict the solution for unseen f(x, y).





### **Operator learning**

**Input-output map**  $\Phi: \mathcal{F} \to \mathcal{U}$   $\mathcal{F}, \mathcal{U}$  are infinite dimensional function space

**Data**  $\{\mathcal{F}_i, \mathcal{U}_i\}_{i=1}^n$   $\mathcal{U}_i = \Phi(\mathcal{F}_i), \mathcal{F}_i \sim \mu \ i. i. d$ 

**Operator learning**  $\Psi: \mathcal{F} \times \Theta \to \mathcal{U}$  such that  $\Psi(., \theta^*) \approx \Phi$ 

**Training**  $\theta^* = \operatorname{argmin}_{\theta} l(\{\mathcal{F}_i, \Psi(\mathcal{U}_i, \theta)\})$ 

Universal Approximation Theorem for Operators  $\mathcal{G}: f \to \mathcal{G}(f), \mathcal{G}(f): y \in \mathbb{R}^d \to \mathbb{R}$ 

# Deep Operator Network (DeepONet)

- Generalized Universal Approximation Theorem for Operator [Chen '95, Lu et al. '19] ٠
- **Branch net**: Input  $\{f(x_i)\}_{i=1}^m$ , output:  $[b_1, b_2, ..., b_p]^T \in \mathbb{R}^p$ **Branch net**: Input  $\{j(x_i)\}_{i=1}^{j=1}, \dots, j_p\}_{i=1}^{T} \in \mathbb{R}^p$  **Trunk net**: Input y, output:  $[t_1, t_2, \dots, t_p]^T \in \mathbb{R}^p$   $\hat{u} = G_{\theta}(f)(y) = \sum_{i=1}^p b_i(f(x_1), f(x_2), \dots, f(x_m)) \cdot tr_i(y)$ branch net trunk net ٠
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### Constructing the DeepONet model





### Transfer learning

- Transfer learning (TL) allows us to learn from a source data distribution a well performing model on a different but related target data distribution
- TL addresses the expense of data acquisition and labelling, potential computational power limitations and dataset distribution mismatches
- Problem setup:

 $\mathcal{D}^{\mathcal{S}} = \{ (x_i^{\mathcal{S}}, y_i^{\mathcal{S}}) \} \text{ labeled data sampled from } P \neq Q$  $\mathcal{D}^{\mathcal{T}} = \{ (x_i^{\mathcal{T}}) \} \text{ (un)labeled data samples from } Q$ 

S: source domain, T: target domain



### Covariate vs conditional shift



$$u_t = \left(\frac{u^2}{2}\right)_x + v u_{xx}.$$



11



### Learning the solution of PDE on multiple domains

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**Conditional**  $P(x_s) = P(x_t)$ shift:  $P(y_s|x_s) \neq P(y_t|x_t)$ 

\* $x_s$ : Model inputs;  $y_s$ : Model outputs

- Learning surrogate models in *isolation* is expensive
- Training a surrogate with very few data can lead to overfitting
- Networks used for similar tasks (datasets) should be similar
- Leverage learned information between source and target models
  - $\checkmark$  Remove the need for big data for every new problem
  - ✓ Accelerate learning by fast fine-tuning of target network

Goswami, S., Kontolati, K., et al. (2022). Nature Machine Intelligence

### Transfer learning approach



# CEOD: Conditional embedding operator discrepancy

Given two datasets:  $\mathcal{D}_p = \{(x_1, y_1), ..., (x_{N_1}, y_{N_1})\},$  $\mathcal{D}_q = \{(x_1, y_1), ..., (x_{N_2}, y_{N_2})\}$  $D_{\text{CEOD}}(\mathcal{D}_p, \mathcal{D}_q) = \left\|\hat{C}_{Y_p|X_p} - \hat{C}_{Y_q|X_q}\right\|_{H^c}^2$ 

$$= \left\| \Phi(Y_p) \left( \mathbf{K}_{X_p X_p} + \lambda N_1 \mathbf{I} \right)^{-1} \mathcal{Y}^{\mathrm{T}}(X_p) - \Phi(Y_q) \left( \mathbf{K}_{X_q X_q} + \lambda N_2 \mathbf{I} \right)^{-1} \mathcal{Y}^{\mathrm{T}}(X_q) \right\|_{HS}^{2}$$

$$= \operatorname{Tr} \left\{ \left( \mathbf{K}_{X_p X_p} + \lambda N_1 \mathbf{I} \right)^{-1} \mathbf{K}_{Y_p Y_p} \left( \mathbf{K}_{X_p X_p} + \lambda N_1 \mathbf{I} \right)^{-1} \mathbf{K}_{X_p X_p} \right\}$$

$$+ \operatorname{Tr} \left\{ \left( \mathbf{K}_{X_q X_q} + \lambda N_2 \mathbf{I} \right)^{-1} \mathbf{K}_{Y_q Y_q} \left( \mathbf{K}_{X_q X_q} + \lambda N_2 \mathbf{I} \right)^{-1} \mathbf{K}_{X_q X_q} \right\}$$

$$- 2 \operatorname{Tr} \left\{ \left( \mathbf{K}_{X_p X_p} + \lambda N_1 \mathbf{I} \right)^{-1} \mathbf{K}_{Y_p Y_q} \left( \mathbf{K}_{X_q X_q} + \lambda N_2 \mathbf{I} \right)^{-1} \mathbf{K}_{X_q X_q} \right\}$$

- Inspired by:  $D_{MMD}(\mathcal{D}_p, \mathcal{D}_q) = \left\| \hat{\mu}_{X_p} \hat{\mu}_{X_q} \right\|_{HS}^2$
- CEOD measures the conditional distribution discrepancy in a reproducing kernel Hilbert space (RKHS)
- Constructs a Hilbert–Schmidt norm of the empirical conditional embedding operators of two distributions
- Based on the theory of kernel embeddings of conditional distributions

 $C_{Y|X}$ : operator of inputs to outputs on a RKHS  $\Phi, \mathcal{Y}$ : embed from original space to RKHS  $\mathbf{K}_{XX'}$ : Gram matrix calculated with a Gaussian kernel k $\lambda$ : regularization term to avoid overfitting

# CEOD: Conditional embedding operator discrepancy

RVS: X, Y Original space  $\Omega_X$ ,  $\Omega_Y$ RKHS feature spaces  $\mathcal{H}, \mathcal{F}$ Given a dataset:  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$ :  $x \in \Omega_X$  $\begin{array}{c} \text{embed} \\ & \stackrel{*}{\varphi(X): \Omega_{X} \to \mathcal{H}} \\ & \psi(Y): \Omega_{Y} \to \mathcal{F} \end{array} \end{array} \left\{ \begin{array}{c} \psi(Y), \varphi(X) \\ & \mu_{Y}, \mathcal{C}_{Y}, \mathcal{C}_{YX} \\ & \mu_{X}, \mathcal{C}_{XY}, \mathcal{C}_{X} \end{array} \right\}$  $\hat{C}_{Y|X} = \hat{C}_{YX}\hat{C}_{XX}^{-1} = \Phi(\mathbf{K} + \lambda N\mathbf{I})^{-1}\mathcal{Y}^{\mathrm{T}}$  $\begin{array}{c}X \sim \mathbb{P}_{X}\\Y \sim \mathbb{P}_{Y}\\(X,Y) \sim \mathbb{P}_{XY}\end{array}\right\} \Phi \coloneqq (\psi(\mathbf{y}_1), \dots, \psi(\mathbf{y}_N))$ where  $\mathcal{Y} \coloneqq (\varphi(\mathbf{x}_1), \dots, \varphi(\mathbf{x}_N))$ conditional  $\mathbf{K} = \mathcal{Y}^{\mathrm{T}} \mathcal{Y}$  Gram matrix conditioning on operator and X = x $\lambda$ : regularization parameter mean embedding Given two datasets  $\mathcal{D}_p$ ,  $\mathcal{D}_q$ :  $C_{Y|X} = C_{YX}C_{XX}^{-1}$ embed  $(Y|X = x) \sim \mathbb{P}_{Y|X=x}$  $\mu_{Y|X=x} = C_{Y|X}\varphi(x)$  $D_{\text{CEOD}}(\mathcal{D}_p, \mathcal{D}_q) = \left\| \hat{C}_{Y_p | X_p} - \hat{C}_{Y_q | X_q} \right\|_{U_c}^2$  $\mathcal{C}_{Y|X}$ : operator  $\mathcal{H} \to \mathcal{F}$ 

\*  $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$ 

15 Klebanov et al. (2020) *SIAM Journal on Mathematics of Data Science* 

### Transfer learning DeepONet loss function

#### Hybrid loss function

$$\mathcal{L}(\theta^{T}) = \lambda_{1}\mathcal{L}_{r}(\theta^{T}) + \lambda_{2}\mathcal{L}_{CEOD}(\theta^{T})$$
$$= \lambda_{1}\frac{\|f_{T}(\mathbf{x}^{tL}) - \mathbf{y}^{tL}\|_{2}}{\|\mathbf{y}^{tL}\|_{2}} + \lambda_{2}\|\hat{\mathcal{C}}_{Y_{tL}|X_{tL}} - \hat{\mathcal{C}}_{Y_{tU}|X_{tU}}\|_{HS}^{2}$$

 $\lambda_1, \lambda_2$ : Trainable coefficients updated through backpropagation<sup>1</sup>

#### **Regression loss**

#### **CEOD** loss

- $\mathcal{D}_t = \{ (\mathbf{x}_i^{tL}, \mathbf{y}_i^{tL}) \}_{i=1}^{N_t}$   $\mathcal{D}_t^L = \{ (\mathbf{x}_{b_1 i}^{tL}, \mathbf{y}_i^{tL}) \}_{i=1}^{N_t}$ •  $\mathcal{D}_{t}^{U} = \{ \left( \mathbf{x}_{b_{1}i}^{tU}, f_{T}(\mathbf{y}_{i}^{tU}) \right) \}_{i=1}^{N_{u}}$ 
  - $\mathbf{x}_{b_1}$ : output of the 1<sup>st</sup> FNN layer of branch net





### Transfer learning applications

Angeligetien	Input Function	Madal Output	Domain Visualization		
		Model Output	Source	Target/s	
	Random input conductivity field	$\nabla . \left( K(\boldsymbol{x}) \nabla h(\boldsymbol{x}) \right) = 1$			geometric domain shift
Darcy Flow	$K(\mathbf{x}) \sim \mathcal{GP}(0, \mathcal{K}(\mathbf{x}, \mathbf{x}'))$ $\mathcal{K}(\mathbf{x}, \mathbf{x}') = \exp\left[-\frac{(\mathbf{x} - \mathbf{x}')^2}{2l^2}\right]$ $l = 0.25, \mathbf{x}, \mathbf{x}' \in [0, 1]^2$	$h(\mathbf{x}) = 0  \forall  \mathbf{x} \in \partial \Omega$ $\mathcal{G}_{\theta} \colon K(\mathbf{x}) \to h(\mathbf{x})$	5	TL4	
Elasticity	Random boundary conditions $f(x) \sim \mathcal{GP}(0, \mathcal{K}(x, x'))$	$\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{f}(\boldsymbol{x}) = 0$ (u, v) = 0 \forall x = 0 $\mathcal{G}_{\theta} : \boldsymbol{f}(\boldsymbol{x}) \to (u, v)$ u: X-Displacement			geometric domain + model
Model	$\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = \exp\left[-\frac{(\boldsymbol{x} - \boldsymbol{x}')^{2}}{2l^{2}}\right]$ $l = 0.12, \boldsymbol{x}, \boldsymbol{x}' \in [0, 1]$	Material properties $E_S = 300 \cdot 10^5$ $E_{T_1} = 410 \cdot 10^3, v_{T_1} = 0.35$ $v_S = 0.3$ $E_{T_2} = 410 \cdot 10^3, v_{T_2} = 0.45$			
Brusselator Diffusion- Reaction System	Random initial condition $h_2(\mathbf{x}) \sim \mathcal{GP}(h_2(\mathbf{x}) \mu(\mathbf{x}), \mathcal{K}(\mathbf{x}, \mathbf{x}'))$ $v(\mathbf{x}, \mathbf{y}, t = 0) = h_2(\mathbf{x}, \mathbf{y}) \ge 0$ $\mathcal{K}(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left[-\frac{(\mathbf{x} - \mathbf{x}')^{\wedge 2}}{2l^2}\right]$ $l_x = 0.12, l_y = 0.4, \sigma^2 = 0.15$	$ \begin{array}{c c} \frac{\partial u}{\partial t} = D_0 \nabla^2 u + a - (1 - b)u + vu^2 \\ \frac{\partial v}{\partial t} = D_1 \nabla^2 v + bu - vu^2 \\ x \in [0,1]^2, t \in [0,1] \\ \mathcal{G}_{\theta}: h_2(x,y) \rightarrow v(x,y,t) \\ \hline \text{Model parameter} \\ \hline b_S = 2.2 \qquad b_{T_1} = 1.7, \\ b_{T_2} = 3.0 \\ \end{array} $	$\begin{array}{c} \begin{array}{c} \begin{array}{c} v(x_{r},y_{r},t) \\ u(x_{r},y_{r},t) \end{array} \end{array}$	TL7	model dynamics shift

# Results: Darcy Flow (TL3)

**Random input** 

Objective:

 $\mathcal{G}: K(\boldsymbol{x}) \to h(\boldsymbol{x})$ 

conductivity field  

$$K(\mathbf{x}) \sim \mathcal{GP}(0, \mathcal{K}(\mathbf{x}, \mathbf{x}')) \qquad \nabla(K(\mathbf{x}) \nabla h(\mathbf{x})) = 1$$

$$\mathcal{K}(\mathbf{x}, \mathbf{x}') = \exp\left[-\frac{(\mathbf{x} - \mathbf{x}')^2}{2l^2}\right] \qquad h(\mathbf{x}) = 0 \quad \forall \quad \mathbf{x} \in \partial\Omega$$

$$l = 0.25, \mathbf{x}, \mathbf{x}' \in [0, 1]^2$$

Undraulia boad

Transfer learning scenario:





# Results: Darcy Flow (TL4)

Random input

conductivity field

 $K(\boldsymbol{x}) \sim \mathcal{GP}(0, \mathcal{K}(\boldsymbol{x}, \boldsymbol{x}'))$ 

 $\mathcal{K}(\boldsymbol{x}, \boldsymbol{x}') = \exp\left[-\frac{(\boldsymbol{x}-\boldsymbol{x}')^2}{2l^2}\right]$  $l = 0.25, \boldsymbol{x}, \boldsymbol{x}' \in [0,1]^2$ 

Objective:

 $\mathcal{G}: K(\boldsymbol{x}) \to h(\boldsymbol{x})$ 

Hydraulic head

$$\nabla . \left( K(\boldsymbol{x}) \nabla h(\boldsymbol{x}) \right) = 1$$
$$h(\boldsymbol{x}) = 0 \quad \forall \quad \boldsymbol{x} \in \partial \Omega$$







#### Representative results of TL-DeepONet for Darcy's problem

### Representative result: Darcy Flow

	$N_t$	TL1	$\mathrm{TL2}$	TL3	$\mathrm{TL4}$
Training DeepONet (source)	2,000	15,260	15,260	15,260	2,261
Training DeepONet (target)	2,000	12,880	18,200	18,080	$3,\!978$
Training TL-DeepONet	$egin{array}{ccc} & 5 & - & 5 \ & 20 & 50 & 100 & 150 & 150 & 200 & 250 & 250 & 0 \end{array}$	$ \begin{array}{r}     -11 \\     129 \\     416 \\     439 \\     459 \\     462 \\     531 \\ \end{array} $	$egin{array}{c} & 10 & 116 \ & 399 \ & 437 \ & 439 \ & 480 \ & 528 \end{array}$	$egin{array}{ccc} & \overline{10} & - & - & - & - & - & - & - & - & - & $	
	$250 \\ 2,000$	$\frac{531}{595}$	528 601	586 653	30. 35

#### **Table**: GPU time (s) for all Darcy flow transfer learning scenarios

### Results: Linear elasticity (TL5)

Objective:Random RHSDisplacement $\mathcal{G}: f(x) \rightarrow [u(x), v(x)]$  $f(x) \sim \mathcal{GP}(0, \mathcal{K}(x, x'))$  $\nabla \cdot \sigma + f(x) = 0$  $\mathcal{K}(x, x') = \exp\left[-\frac{(x-x')^2}{2l^2}\right]$  $u(x) = v(x) = 0 \ \forall x = 0$  $l = 0.12, x, x' \in [0,1]^2$ 





# Results: Limitations of TL-DeepONet



	$N_t$	$L_2$ (%)			
		$u(oldsymbol{x})$	$v(oldsymbol{x})$	time $(s)$	
Training DeepONet	1,900	$2.30 \pm 0.49$	$3.22 \pm 0.48$	10,060	
Training DeepONet (target)	1,900	$2.72\pm0.26$	$1.92\pm0.41$	11,750	
Training TL-DeepONet	$-\frac{5}{5}$ - 20 50 100 150 200 250	$\begin{array}{c} -\overline{60.28} \pm \overline{1.95} \\ 29.14 \pm 0.31 \\ 16.4 \pm 2.01 \\ 11.37 \pm 0.34 \\ 9.66 \pm 0.26 \\ 5.52 \pm 0.20 \\ 4.08 \pm 0.06 \\ 2.82 \pm 0.20 \end{array}$	$\begin{array}{c} \overline{57.48} \pm \overline{2.54} \\ 21.42 \pm 3.20 \\ 18.72 \pm 1.18 \\ 14.15 \pm 0.96 \\ 11.95 \pm 0.61 \\ 10.94 \pm 0.20 \\ 9.18 \pm 0.14 \\ 7.80 \pm 0.21 \end{array}$	$     \begin{array}{r}       - & - & - \\       18 & - & - \\       148 & 25 & \\       44 & \\       116 & \\       384 & \\       480 & \\       512 & \\     \end{array} $	
	$1,\!900$	$3.82\pm0.20$	$7.89\pm0.21$	512	



- Different internal, external boundaries and material properties;
- Predicted displacements field deviates significantly with the response predicted by training DeepONet from scratch

1 Error ×10<sup>-8</sup> 10 8 6 4





- Learn operators on multiple PDE domains via transfer learning and treat trained models as reusable building blocks
- TL-DeepONet:
  - Performs well under small-data regimes
  - TL-DeepONet accelerates learning via fine-tuning pre-trained models
  - Enhances generalizability in neural operators
- Code availability: <u>https://github.com/katiana22/TL-DeepONet.git</u>





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# The team





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#### Computing support:



@Brown

Advanced Research Computing at Hopkins

RockFish @JHU





Dr. Michael Shields Associate Professor Johns Hopkins University



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### Positions available Ph.D. -2 (starting Spring) Postdocs – 1 (immediately) in the Department of Civil and Systems Engineering at Johns Hopkins University Topics: SciML for materials and mechanics Email: somdatta89@gmail.com

# Thank you!