Learning Solution Operators For PDEs *** Algorithms, Analysis and Applications

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Operator Learning

Supervised Learning

Determine $\Psi^{\dagger}: \mathcal{U} \to \mathcal{V}$ from samples

$$\{u_n, \Psi^{\dagger}(u_n)\}_{n=1}^N, \quad u_n \sim \mu.$$

Probability measure μ supported on \mathcal{U} .

In standard supervised learning $\mathcal{U} = \mathbb{R}^{d_X}$ and $\mathcal{V} = \mathbb{R}^{d_y}$ (regression) or $\mathcal{V} = \{1, \cdots K\}$ (classification).

Supervised Learning Of Operators

Separable Banach spaces \mathcal{U}, \mathcal{V} of vector-valued functions:

$$\mathcal{U} = \{ u : D_u \to \mathbb{R}^{d_i} \}, \quad D_u \subseteq \mathbb{R}^{d_u}$$
$$\mathcal{V} = \{ v : D_v \to \mathbb{R}^{d_o} \}, \quad D_v \subseteq \mathbb{R}^{d_v}.$$

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Operator Learning

Training

Consider a family of parameterized functions from ${\cal U}$ into ${\cal V}$:

 $\Psi: \mathcal{U}\times \Theta \mapsto \mathcal{V}.$

Here $\Theta \subseteq \mathbb{R}^p$ denotes the parameter space.

$$\mu_{N} = \frac{1}{N} \sum_{n=1}^{N} \delta_{u_{n}}, \quad \mathsf{RE}(v, w) = \frac{\|v - w\|_{\mathcal{V}}}{\max\{1, \|v\|_{\mathcal{V}}\}},$$
$$\theta^{*} = \operatorname{argmin}_{\theta \in \Theta} \mathcal{R}_{N}(\theta), \quad \mathcal{R}_{N}(\theta) := \mathbb{E}^{u \sim \mu_{N}} \mathsf{RE}(\Psi^{\dagger}(u), \Psi(u; \theta)).$$

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Example (Porous Medium Flow)

Darcy Law

Mass conservation Boundary condition $-\nabla \cdot (a\nabla v) = f, \quad x \in D$ $v = 0, \quad x \in \partial D$

Operator Of Interest

Parametric Dependence $\Psi^{\dagger}: a \mapsto v$

Example (Porous Medium Flow)

Input-Output





Example (Porous Medium Flow): Discretize Then Learn



Example (Porous Medium Flow): Learn Then Discretize



Bhattacharya et al 2021 [2]

Examples: (Homogenized Constitutive Models)

Material Properties Dependence

- \mathcal{U} : material properties $A(\cdot)$.
- $\triangleright \mathcal{V}$: stress σ .

•
$$\sigma = \Psi^{\dagger}(A)(\nabla u + \nabla u^{\top}).$$

• Approximate $\Psi^{\dagger} \approx \Psi(\cdot; \theta^{\star})$

History Dependence

• \mathcal{U} : time histories of strain $\{\nabla u\}$.

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• \mathcal{V} : time histories of stress $\{\sigma\}$.

$$\blacktriangleright \ \{\sigma\} = \Psi^{\dagger}(\{\nabla u\}).$$

• Approximate $\Psi^{\dagger} \approx \Psi(\cdot; \theta^{\star})$

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Finding Latent Structure



$$\begin{aligned} & G_{\mathcal{U}} \circ F_{\mathcal{U}} \approx \mathsf{Id} \\ & G_{\mathcal{V}} \circ F_{\mathcal{V}} \approx \mathsf{Id} \\ & G_{\mathcal{V}} \circ \varphi \circ F_{\mathcal{U}} \approx \Psi^{\dagger} \end{aligned}$$

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PCA-NET

Architecture Bhattacharya, Hosseini, Kovachki and AMS '19 [2]

$$\Psi_{PCA}(u;\theta)(x) = \sum_{j=1}^m \alpha_j(Lu;\theta)\psi_j(x), \quad \forall u \in \mathcal{U} \qquad x \in D_v.$$

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Details

- $\{\phi_j\}$ are PCA basis functions under μ .
- $Lu = \{\langle \phi_j, u \rangle\}$ maps to PCA coefficients under μ .
- $\{\psi_j\}$ are PCA basis functions under $(\Psi^{\dagger})^{\sharp}\mu$.
- $\{\alpha_j\}$ are finite dimensional neural networks.

DEEPONET Shallow approximation of functionals (Chen and Chen [5]) made deep

Architecture Lu, Jin, Pang, Zhang, and Karniadakis'19 [18]

$$\Psi_{DEEP}(u;\theta)(x) = \sum_{j=1}^{m} \alpha_j(Lu;\theta_\alpha)\psi_j(y;\theta_\psi), \quad \forall u \in \mathcal{U} \qquad x \in D_{\nu}.$$

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Details

- Lu maps to linear functionals on U.
- e.g. PCA coefficients under μ ; or pointwise $\{u(x_{\ell})\}$.
- $\{\alpha_j, \psi_j\}$ are finite dimensional neural networks.

$$\blacktriangleright \ \theta = (\theta_{\alpha}, \theta_{\psi}).$$

Fourier Neural Operator (FNO) DNN (Goodfellow et al [7]) Extended to Operators

Architecture Li, Kovachki, Azizzadenesheli, Liu, Bhattacharya, AMS and Anandkumar et al '20 [16, 11]

 $\mathcal{U}=\mathcal{V} ~ \mathsf{Hilbert}$

$$\begin{split} \Psi_{FNO}(u;\theta) &= \mathcal{Q} \circ \mathcal{L}_L \circ \cdots \mathcal{L}_2 \circ \mathcal{L}_1 \circ \mathcal{R}(u), \, \forall u \in \mathcal{U}, \\ \mathcal{L}_I(v)(x;\theta) &= \sigma \big(W_I v(x) + b_I + \mathcal{K}(v)(x;\gamma_I) \big), \\ \mathcal{K}(v)(x;\gamma) &= \sum_{m=1}^M \alpha_m \big(\gamma(m) \big) \langle \mathsf{f}_m, v \rangle_{\mathcal{U}^{\otimes d_c}} \mathsf{g}_m(x). \end{split}$$

Details

- Q, R pointwise NNs or linear transformations.
- (W_l, b_l) define pointwise affine transformations.
- K eg FFT as convolutional integral operator.
- θ collects parameters from previous three bullets.

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Universal Approximation (Latent) over compact sets

Definition

A Banach space has the **approximation property (AP)** if every compact operator is a limit of finite-rank operators.

Theorem 1 Kovacvhki '22 [10, 11]

Assume

U, V Banach spaces with the AP.

• $\Psi^{\dagger}: \mathcal{U} \to \mathcal{V}$ continuous, $K \subset \mathcal{U}$ compact.

For any $\epsilon > 0 \exists$ bounded linear $F_{\mathcal{U}} : \mathcal{U} \to \mathbb{R}^{d_{\mathcal{U}}}$, $G_{\mathcal{V}} : \mathbb{R}^{d_{\mathcal{V}}} \to \mathcal{V}$, and a continuous map $\varphi \in C(\mathbb{R}^{d_{\mathcal{U}}}; \mathbb{R}^{d_{\mathcal{V}}})$ such that

$$\sup_{u\in K} \|\Psi^{\dagger}(u) - (G_{\mathcal{V}}\circ\varphi\circ F_{\mathcal{U}})(u)\|_{\mathcal{V}} \leq \epsilon.$$

Universal Approximation (Latent) Bochner integration

Theorem 2 Kovacvhki '22 [10, 11]

Assume

- \mathcal{U} Banach space with AP, \mathcal{V} separable Hilbert space.
- μ probability measure on \mathcal{U} .

•
$$\Psi^{\dagger} \in L^{p}_{\mu}(\mathcal{U}; \mathcal{V})$$
 for $1 \leq p < \infty$.

For any $\epsilon > 0 \exists$ bounded linear $F_{\mathcal{U}} : \mathcal{U} \to \mathbb{R}^{d_{\mathcal{U}}}$, $G_{\mathcal{V}} : \mathbb{R}^{d_{\mathcal{V}}} \to \mathcal{V}$, and a continuous map $\varphi \in C(\mathbb{R}^{d_{\mathcal{U}}}; \mathbb{R}^{d_{\mathcal{V}}})$ such that

$$\|\Psi^{\dagger} - G_{\mathcal{V}} \circ \varphi \circ F_{\mathcal{U}}\|_{L^{p}_{\mu}(\mathcal{U};\mathcal{V})} \leq \epsilon.$$

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Lanthaler, Mishra and Karniadakis '21 [14] (DeepONet and complexity, NSE)

Lanthaler '23 [12] (PCA-Net and complexity, Darcy and NSE)

Marcati and Schwab '23 [19] (Complexity estimates, Darcy)

Lanthaler and AMS '23 [15] (Complexity estimates, Hamilton-Jacobi)

Universal Approximation (FNO)

Theorem 3 Lanthaler, Li and AMS '23 [13]

Assume

 $\mathcal{U} = C(\overline{D}, \mathbb{R}^d).$ $\mathcal{V} = C(\overline{D}, \mathbb{R}^{d'}).$

• $\Psi^{\dagger}: \mathcal{U} \to \mathcal{V}$ continuous, $K \subset \mathcal{U}$ compact.

For any L, M > 0 and any $\epsilon > 0 \exists$ an FNO $\Psi(\cdot; \theta^*) : U \to V$ such that

$$\sup_{u\in K} \|\Psi^{\dagger}(u) - \Psi(u;\theta)\|_{\mathcal{V}} \leq \epsilon.$$

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Kovachki, Lanthaler and Mishra '21 [9] (Complexity, FNO)

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Multiscale Problem

Canonical Elliptic Multiscale Problem

$$\begin{aligned} -\nabla \cdot \left(A^{\epsilon} \nabla u^{\epsilon}\right) &= f, \quad x \in \Omega \\ u^{\epsilon} &= 0, \quad x \in \partial \Omega \\ A^{\epsilon}(x) &= A\left(\frac{x}{\epsilon}\right), \quad A \in \mathcal{U} := L^{\infty}(\mathbb{T}^{d}, \mathbb{R}^{d \times d}). \end{aligned}$$

Standing Asssumption on A

$$\begin{split} PD_{\alpha,\beta} = & \{ A \in L^{\infty}(\mathbb{T}^d; \mathbb{R}^{d \times d}) : \\ & \forall (y,\xi) \in \mathbb{T}^d \times \mathbb{R}^d, \; \alpha |\xi|^2 \leq \langle \xi, A(y)\xi \rangle \leq \beta |\xi|^2 \}. \end{split}$$

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Operator Learning

Homogenized Elliptic Problem; $u_0 \approx u^{\epsilon}$

$$egin{aligned} -
abla \cdot (A_0
abla u_0) &= f, \quad x \in \Omega \ u_0 &= 0, \quad x \in \partial \Omega \ A_0(x) &= A_0, \quad ext{constant.} \end{aligned}$$

$$egin{aligned} -
abla_y \cdot (
abla_y \chi \, A) &=
abla_y \cdot A, \quad y \in \mathbb{T}^d, \ A_0 &= \int_{\mathbb{T}^d} \left(A(y) + A(y)
abla \chi(y)^T
ight) \, dy \end{aligned}$$

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Universal Approximation (Cell Problem Solution Operator)

Goal: Supervised Learning (FNO)

Bhattacharya, Kovachki, Rajan, AMS, Trautner '23 [3]

• Learn map
$$A(\cdot) \in \mathcal{U} \mapsto \chi(\cdot) \in \mathcal{V} = H^1_{\mathrm{per}}(\mathbb{T}^d, \mathbb{R}^d).$$

How to choose U?

Theorem 4 Bhattacharya, Kovachki, Rajan, AMS, Trautner '23 [3]

Define the mapping $\Psi^{\dagger}: PD_{\alpha,\beta} \to \dot{H}^{1}(\mathbb{T}^{d}; \mathbb{R}^{d})$ from the solution map $A \mapsto \chi$ given by

$$-
abla_y \cdot (
abla_y \chi A) =
abla_y \cdot A, \quad y \in \mathbb{T}^d.$$

Then, for any $\epsilon > 0$ and $K \subset PD_{\alpha,\beta}$ compact in $L^2(\mathbb{T}^d; \mathbb{R}^{d \times d})$, there exists an FNO $\Psi(\cdot; \theta^*) : K \to \dot{H}^1(\mathbb{T}^d; \mathbb{R}^d)$ such that

$$\sup_{A\in K} \|\Psi^d(A) - \Psi(A;\theta^*)\|_{\dot{H}^1} < \epsilon.$$

Varying Microstructures



 $\mathcal{K} \subset \mathsf{BV}(\mathbb{T}^d; \mathbb{R}^{d \times d}) \cap \mathcal{PD}_{\alpha, \beta} \Subset L^2(\mathbb{T}^d; \mathbb{R}^{d \times d}).$

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Learning Error for Voronoi Microstructure



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Test Error versus Data Size



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Test Error versus Model Size



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Big Picture

Multiscale Problem Pavliotis and AMS '08 [20][Ch12]

Displacement $u^{\epsilon}(x, t)$, stress $\sigma^{\epsilon}(x, t)$, $0 < \epsilon \ll 1$. F=MA:

$$\rho \,\partial_t^2 u^\epsilon = \nabla \cdot (\sigma^\epsilon) + f, \quad \sigma^\epsilon = \Psi^\epsilon \left(\{ \nabla u^\epsilon \}, \frac{x}{\epsilon} \right).$$

Homogenized Problem Bensoussan, Lions, Papanicolaou [1]

Approximate $u^{\epsilon} = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \dots$

Determine map Ψ , so that small scales are removed in u_0 . F=MA:

$$\rho \partial_t^2 u_0 = \nabla \cdot (\sigma) + f, \quad \sigma = \Psi(\{\nabla u_0\}).$$

Operator Learning

- \mathcal{U} histories of strain $\{\nabla u_0\}$; Vhistories of stress $\{\sigma\}$.
- Approximate $\Psi \approx \Psi_{NN}$

Viscoelasticity | Francfort and Suquet '86 [6]

Quasi-Static Viscoelasticity Multiscale Problem

$$\begin{aligned} -\nabla \cdot (\sigma^{\epsilon}) &= f, \quad x \in \Omega\\ \sigma^{\epsilon} &= \nu^{\epsilon} \partial_t \nabla u^{\epsilon} + E^{\epsilon} \nabla u^{\epsilon}\\ E^{\epsilon}(x) &= E\left(\frac{x}{\epsilon}\right), \quad \nu^{\epsilon}(x) = \nu\left(\frac{x}{\epsilon}\right), \quad E, \nu : \mathbb{T}^d \to \mathbb{R}. \end{aligned}$$

Laplace Transform, Homogenize, Invert

$$egin{aligned} -
abla \cdot (\overline{\sigma}^\epsilon) &= f, \quad x \in \Omega \ \overline{\sigma}^\epsilon &= (s
u^\epsilon + E^\epsilon)
abla \overline{u}^\epsilon. \end{aligned}$$

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Introduces memory.

Viscoelasticity II Bhattacharya, Liu, AMS, Trautner '22 [4]

Theorem (Piecewise-Constant Homogenization: Memory)

In piecewise-constant case and in dimension d = 1 homogenized equation for u_0 is Markovian:

$$\begin{aligned} -\nabla \cdot (\sigma) &= f, \quad x \in \Omega, \\ \sigma &= \nu' \partial_t \nabla u_0 + E' \nabla u_0 + \langle \mathbb{1}, r \rangle \\ \partial_t r_\ell &= -\alpha_\ell r_\ell + \beta_\ell \nabla u_0, \quad \ell \in \{1, 2, \cdots, L\}, \end{aligned}$$

for some choice of $E' \in \mathbb{R}_+$, $\nu' \in \mathbb{R}_+$, $\alpha \in \mathbb{R}_+^L$, $\beta \in \mathbb{R}^L$, $L \in \mathbb{Z}_+$.

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Homogenization introduces memory.

- ln d = 1 (approximate) Markovian structure.
- Dimension d > 1 ?

Viscoelasticity III: Operator Learning

True Solution Map

Let $\Psi: \mathcal{U} \to \mathcal{V}$ be the map such that the homogenized constitutive relation is

$$\sigma = \Psi(\{\nabla u_0\}).$$

Goal: Supervised Learning (RNO-NET)

Learn map $\Psi_{\textit{RNO}}: \mathcal{U} \rightarrow \mathcal{V}$ approximating Ψ with the form

$$\sigma = F \left(\nabla u_0, \partial_t \nabla u_0, r \right)$$
$$\partial_t r = G(r, \nabla u_0), \quad r(0) = 0$$

RNO – Recurrent neural operator.

Dimension of memory variable *r* has to be learned.

Viscoelasticity IV: Learning the Constitutive Map



Figure: Viscoelasticity: trained model performs well on test samples

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Viscoelasticity V: Choosing the Number of Hidden Variables



Figure: Absolute L^2 error of RNNs trained with different numbers of hidden variables on different piecewise-constant viscoelastic materials.

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Viscoelasticity VI: Time Discretization Invariance



Figure: Viscoelasticity models trained with and without access to the strain rate variable: prefered model exhibits more invariance to time discretization of test trajectories

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Conclusions

- 1. Algorithms:
 - define on function space;
 - then learn;
 - leads to models which transfer between discretizations.
- 2. Analysis:
 - universal approximation theory well-developed;
 - complexity (cost verus error) incompletely understood;

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- what solution is found via optimization?
- 3. Applications:
 - cheap surrogates;
 - scientific discovery;
 - constitutive laws.

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Plasticity | Liu, Kovachki, Li, Azizzadenesheli, Anandkumar, AMS, Bhattacharya '22 [17]

Plasticity Multiscale Problem

$$\begin{split} \rho \, \partial_t^2 u^\epsilon &= \nabla \cdot \sigma^\epsilon + f, \quad x \in \Omega \\ \partial_t \xi^\epsilon &= \mathcal{K}(\xi^\epsilon, \nabla u^\epsilon), \quad x \in \Omega \\ \sigma^\epsilon &= \Psi^\epsilon \Big(\nabla u^\epsilon, \xi^\epsilon, \frac{x}{\epsilon} \Big) \end{split}$$

Plasticity II

Homogenized Plasticity Problem

$$\rho \,\partial_t^2 u_0 = \nabla \cdot \sigma_0 + f, \quad x \in \Omega$$
$$\sigma_0 = \Psi \Big(\{ \nabla u_0 \} \Big)$$

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Plasticity III: Operator Learning

Goal: Supervised Learning (PCA-NET)

Learn map $\Psi_{PCA} : \mathcal{U} \to \mathcal{V}$ approximating Ψ . In particular causality must be learned.

Goal: Supervised Learning (RNO-NET)

Learn map $\Psi_{\textit{RNO}}: \mathcal{U} \rightarrow \mathcal{V}$ approximating Ψ with the form

$$\sigma = F \left(\nabla u_0, \partial_t \nabla u_0, r \right)$$
$$\partial_t r = G(r, \nabla u_0), \quad r(0) = 0.$$

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Plasticity IV: Learning the Constitutive Map



Figure: Viscoplasticity: Trained model performs well on test samples. Left: Input strains. Right: Output truth and approximation.

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Plasticity V: Choosing the Number of Hidden Variables



Figure: Viscoplasticity: 3D polycrystal (different hidden variable counts)

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Plasticity VI: Time Discretization Invariance



Figure: Models with viscoplastic (VP) and elasto-viscoplastic (E-VP) architecture trained on data from an E-VP material: prefered model exhibits more time discretization invariance

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Learning Error for Varying Microstructures (I)



Smooth Microstructure

Star Inclusion Microstructure



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Learning Error for Varying Microstructures (II)



Square Inclusion Microstructure

Voronoi Microstructure



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