A variationally mimetic operator network

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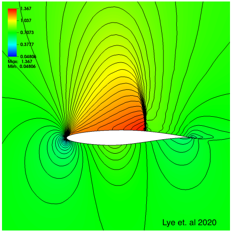
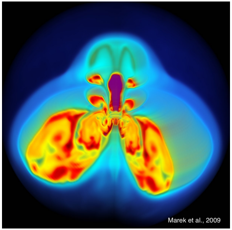
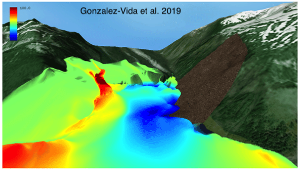






- Problems of interest solved using finite difference/volume, finite element, spectral methods, ...
- Many-query applications need many calls to the solver: e.g.
  - Uncertainty quantification
  - PDE-constrained optimization
  - Inverse problems
- Single solve expensive for large-scale applications $\rightarrow$ multiple solves $\mathcal{O}(10^5)$ prohibitively expensive!
- Need to design efficient, robust surrogates.
- Recent interest in deep learning-based surrogates $\rightarrow$ focus of this talk!

Outline

- Deep learning with neural networks
- Solving PDEs using deep learning
- **Var**iationally **Mi**metic **O**perator **N**etwork (VarMiON)
- Error estimates
- Numerical results
- Conclusion

A neural network is a parametrized mapping

$$NN_{\boldsymbol{\psi}} : \Omega_x \to \Omega_y$$

typically formed by alternating composition

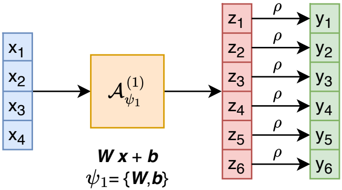
$$NN_{\boldsymbol{\psi}} := \rho \circ \mathcal{A}^{(L+1)}_{\boldsymbol{\psi}_{L+1}} \circ \rho \circ \mathcal{A}^{(L)}_{\boldsymbol{\psi}_L} \circ \rho \circ \mathcal{A}^{(L-1)}_{\boldsymbol{\psi}_{L-1}} \circ \cdots \circ \rho \circ \mathcal{A}^{(1)}_{\boldsymbol{\psi}_1}$$

where

$\boldsymbol{\psi} = \{\boldsymbol{\psi}_k\}_{k=1}^{L} \longrightarrow$ trainable weights and biases of the network

$\mathcal{A}^{(k)}_{\boldsymbol{\psi}_k} \longrightarrow$ parametrized affine transformation

$\rho \longrightarrow$ non-linear activation function



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$$\begin{aligned} \boldsymbol{\psi} = \{\boldsymbol{\psi}_k\}_{k=1}^{L} &\longrightarrow \text{trainable weights and biases of the network} \\ \mathcal{A}^{(k)}_{\boldsymbol{\psi}_k} &\longrightarrow \text{parametrized affine transformation} \\ \rho &\longrightarrow \text{non-linear activation function} \end{aligned}$$

Usage:

- Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be related in some manner, say $\boldsymbol{y} = \mathcal{F}(\boldsymbol{x})$.
- We are only given $\mathcal{S} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^{N}$.
- $NN_{\boldsymbol{\psi}}$ can be used to learn $\mathcal{F}$.

Consider a suitable measure

$$\mu : \Omega_x \times \Omega_y \times \Omega_x \times \Omega_y \to \mathbb{R}$$

s.t. $\mu(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}, NN_{\boldsymbol{\psi}}(\boldsymbol{x}))$ is the error/discrepancy between $(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{S}$ and $(\boldsymbol{x}, NN_{\boldsymbol{\psi}}(\boldsymbol{x}))$.

Define the loss/objective function

$$\Pi(\boldsymbol{\psi}) = \frac{1}{N} \sum_{i=1}^{N} \mu(\boldsymbol{x}_i, \boldsymbol{y}_i, \boldsymbol{x}_i, NN_{\boldsymbol{\psi}}(\boldsymbol{x}_i))$$

Solve the optimization problem

$$\boldsymbol{\psi}^* = \arg\min_{\boldsymbol{\psi}} \Pi(\boldsymbol{\psi})$$

Then $NN_{\boldsymbol{\psi}^*} \approx \mathcal{F}$

Also need to tune network hyper-parameters:
• Width • Depth (L) • Activation function ρ • Optimizer
• Loss function • Dataset

Solving PDEs using deep learning

Consider the generic PDE:

$$\mathcal{L}(u(\boldsymbol{x})) = f(\boldsymbol{x}), \qquad \forall\, \boldsymbol{x} \in \Omega$$

- Solution approximated by a network $\widehat{u}(\boldsymbol{x};\boldsymbol{\psi})$ with parameters $\boldsymbol{\psi}$.
- Minimize PDE residual at collocation points $\{\boldsymbol{x}_i\}$ (Lagaris et al., 2000): Solve

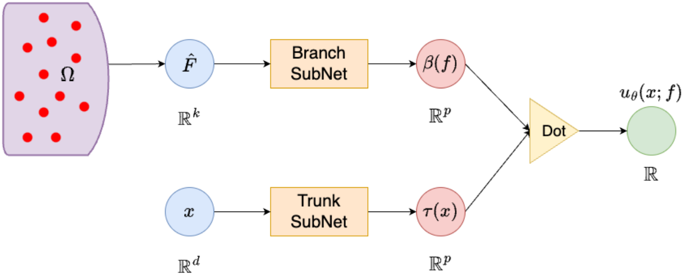
$$\boldsymbol{\psi}^* = \arg\min_{\boldsymbol{\psi}} \Pi(\boldsymbol{\psi}), \quad \Pi(\boldsymbol{\psi}) = \frac{1}{N}\sum_{i=1}^{N} \|\mathcal{L}(\widehat{u}(\boldsymbol{x}_i;\boldsymbol{\psi})) - f(\boldsymbol{x}_i)\|^2$$

- Rediscovered as Physics Informed Neural Nets (PINNs) with deeper structures (Raissi et al., 2019).
- However, solves one instance of the PDE – must be retrained if f changes.

We are interested in approximating the solution operator

$$\mathcal{S} : \mathcal{F} \longrightarrow \mathcal{V}, \qquad \mathcal{S}(f) = u(.; f)$$

- Network-based operator learning with shallow networks [Chen & Chen, 1995].
- DeepONets: extension to deeper architectures [Lu et al., 2021]
- Comprise two subnetworks: the **trunk** (basis) and the **branch** (basis).



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- Neural operators – an alternate strategy to approximate $\mathcal{S}$
- Come in many flavors: Fourier Neural Operators [Li et al., 2020], Graph Kernel Net [Li et al., 2020], PCA-NET [Bhattacharya et al., 2021], ...

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- This talk: Operator Networks that mimic (approximate) variational form* of the PDE.

[* Variationally Mimetic Operator Networks; Patel, Ray, Abdelmalik, Hughes, Oberai; CMAME, 2024]

- Consider a generic linear elliptic PDE:

$$\begin{aligned}
\mathcal{L}(u(\boldsymbol{x});\theta(\boldsymbol{x})) &= f(\boldsymbol{x}), && \forall\, \boldsymbol{x} \in \Omega, \\
\mathcal{B}(u(\boldsymbol{x});\theta(\boldsymbol{x})) &= \eta(\boldsymbol{x}), && \forall\, \boldsymbol{x} \in \Gamma_\eta, \\
u(\boldsymbol{x}) &= 0, && \forall\, \boldsymbol{x} \in \Gamma_g,
\end{aligned}$$

  where $f \in \mathcal{F} \subset L^2(\Omega)$, $\eta \in \mathcal{N} \subset L^2(\Gamma_\eta)$, $\theta \in \mathcal{T} \subset L^\infty(\Omega)$.

- The variational formulation: find $u \in \mathcal{V} \subset H^1_g$ such that $\forall\, w \in \mathcal{V}$,

$$a(w, u; \theta) = (w, f) + (w, \eta)_{\Gamma_\eta}.$$

- The solution operator is

$$\begin{aligned}
\mathcal{S} : \mathcal{X} = \mathcal{F} \times \mathcal{T} \times \mathcal{N} &\longrightarrow \mathcal{V} \subset H^1_g \\
(f, \theta, \eta) &\mapsto u(.; f, \theta, \eta)
\end{aligned}$$

  This mapping can be non-linear in θ.

Discrete weak formulation

- Evaluate approximate solution in finite-dimensional space $\mathcal{V}^h = \text{span}\{\phi_i(\boldsymbol{x}) : 1 \leq i \leq q\}$.

- Discrete weak formulation: find $u^h \in \mathcal{V}^h$ such that $\forall\ w^h \in \mathcal{V}^h$,

$$a(w^h, u^h; \theta^h) = (w^h, f^h) + (w, \eta^h)_{\Gamma_\eta}.$$

- Any function $v^h \in \mathcal{V}^h$ can be written as

$$v^h(\boldsymbol{x}) = \boldsymbol{V}^\top \boldsymbol{\Phi}(\boldsymbol{x}), \quad \boldsymbol{V} = (v_1, \cdots, v_q)^\top, \quad \boldsymbol{\Phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \cdots, \phi_q(\boldsymbol{x}))^\top.$$

  Plugging this into discrete weak form gives...

- Linear system of equations,

$$\boldsymbol{K}(\theta^h)\boldsymbol{U} = \boldsymbol{M}\boldsymbol{F} + \widetilde{\boldsymbol{M}}\boldsymbol{N}$$

where the matrices are given by

$$K_{ij}(\theta^h) = a(\phi_i, \phi_j; \theta^h), \quad M_{ij} = (\phi_i, \phi_j), \quad \widetilde{M}_{ij} = (\phi_i, \phi_j)_{\Gamma_\eta} \quad 1 \leq i, j \leq q.$$

- Discrete solution operator is

$$\begin{aligned} \mathcal{S}^h : \mathcal{X}^h = \mathcal{F}^h \times \mathcal{T}^h \times \mathcal{N}^h &\longrightarrow \mathcal{V}^h \\ (f^h, \theta^h, \eta^h) &\mapsto u^h(.; f^h, \theta^h, \eta^h) = \boldsymbol{B}(f^h, \eta^h, \theta^h)^\top \boldsymbol{\Phi} \end{aligned}$$

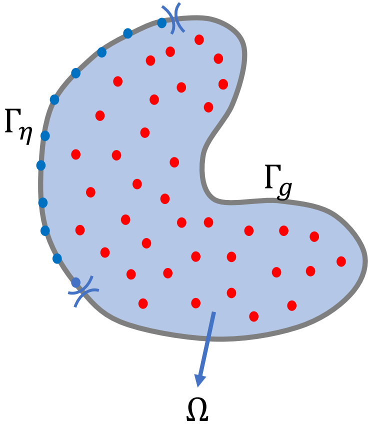
where

$$\boldsymbol{B}(f^h, \theta^h, \eta^h) = \boldsymbol{U} = \boldsymbol{K}^{-1}(\theta^h)(\boldsymbol{M}\boldsymbol{F} + \widetilde{\boldsymbol{M}}\boldsymbol{N}).$$

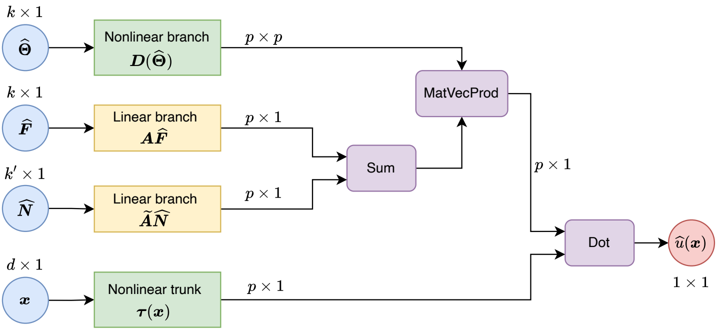
VarMiON will mimic this structure!

Evaluate (f, θ, η) at some fixed **sensor nodes** to get the discrete sample vectors

$$\widehat{\boldsymbol{F}} = (f(\widehat{\boldsymbol{x}}_1), \cdots, f(\widehat{\boldsymbol{x}}_k))^\top, \quad \widehat{\boldsymbol{\Theta}} = (\theta(\widehat{\boldsymbol{x}}_1), \cdots, \theta(\widehat{\boldsymbol{x}}_k))^\top, \quad \widehat{\boldsymbol{N}} = (\eta(\widehat{\boldsymbol{x}}_1^b), \cdots, \eta(\widehat{\boldsymbol{x}}_{k'}^b))^\top$$



The network is comprises several sub-networks with latent dimension p:



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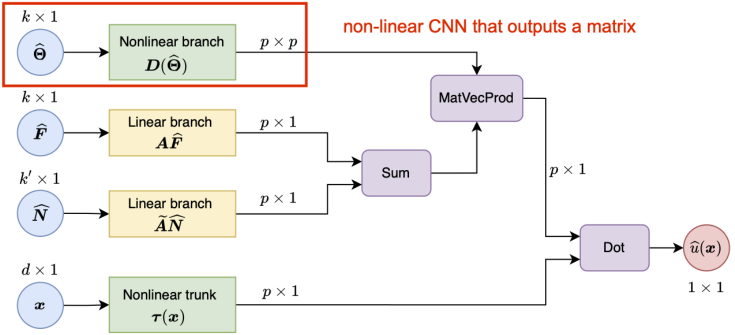
- Non-linear branch net: $\widehat{\boldsymbol{\Theta}} \mapsto \boldsymbol{D}(\widehat{\boldsymbol{\Theta}}) \in \mathbb{R}^{p \times p}$



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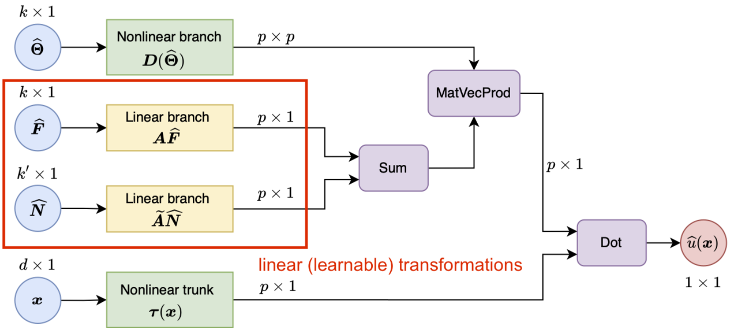

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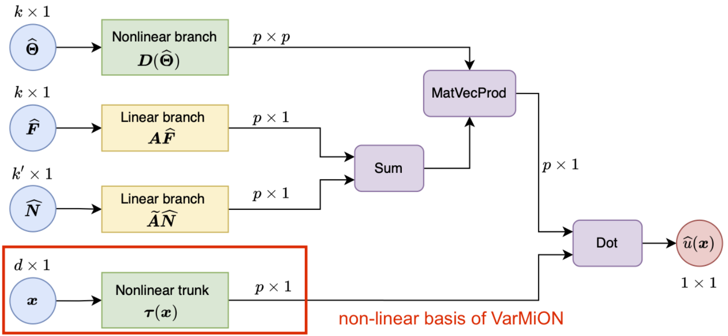
- Two linear branches with learnable matrices $\boldsymbol{A}, \widetilde{\boldsymbol{A}}$
- Non-linear trunk (basis of VarMiON): $\boldsymbol{x} \mapsto \boldsymbol{\tau}(\boldsymbol{x}) = (\tau_1(\boldsymbol{x}), \cdots \tau_p(\boldsymbol{x}))^\top$

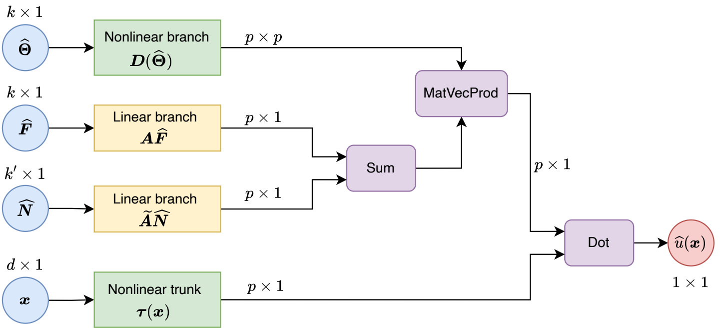


VarMiON operator is

$$\widehat{\mathcal{S}} : \mathbb{R}^k \times \mathbb{R}^k \times \mathbb{R}^{k'} \longrightarrow \mathcal{V}^\tau = \text{span}\{\tau_i(\boldsymbol{x}) : 1 \leq i \leq p\}$$
$$(\widehat{\boldsymbol{F}}, \widehat{\boldsymbol{\Theta}}, \widehat{\boldsymbol{N}}) \mapsto \widehat{u}(.; \widehat{\boldsymbol{F}}, \widehat{\boldsymbol{\Theta}}, \widehat{\boldsymbol{N}}) = \boldsymbol{\beta}(f^h, \eta^h, \theta^h)^\top \boldsymbol{\tau}$$

where

$$\boldsymbol{\beta}(\widehat{\boldsymbol{F}}, \widehat{\boldsymbol{\Theta}}, \widehat{\boldsymbol{H}}) = \boldsymbol{D}(\widehat{\boldsymbol{\Theta}})(\boldsymbol{A}\widehat{\boldsymbol{F}} + \widetilde{\boldsymbol{A}}\widehat{\boldsymbol{N}}).$$



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Compare this to the discrete solution operator:

$$\mathcal{S}^h : \mathcal{F}^h \times \mathcal{T}^h \times \mathcal{N}^h \longrightarrow \mathcal{V}^h$$
$$(f^h, \theta^h, \eta^h) \mapsto u^h(.; f^h, \theta^h, \eta^h) = \boxed{\boldsymbol{B}(f^h, \eta^h, \theta^h)^\top \boldsymbol{\Phi}}$$

where

$$\boldsymbol{B}(f^h, \theta^h, \eta^h) = \boxed{\boldsymbol{K}^{-1}(\theta^h)(\boldsymbol{M}\boldsymbol{F} + \widetilde{\boldsymbol{M}}\boldsymbol{N})}.$$

In comparison with the variational formulation

- Can prove $\boldsymbol{D}$ is the reduced order counterpart of $\boldsymbol{K}^{-1}$ $(p \ll q)$
- While the basis $\boldsymbol{\Phi}$ are fixed, $\boldsymbol{\tau}$ are learned from training data.

In comparison with a vanilla DeepONet

- DeepONet typically has a single nonlinear branch for inputs.
- VarMiON explicitly constructs matrix operators. DeepONet does not.

1. For $1 \leq j \leq J$, consider distinct samples $(f_j, \theta_j, \eta_j) \in \mathcal{X}$.
2. Obtain the discrete approximations $(f_j^h, \theta_j^h, \eta_j^h) \in \mathcal{X}^h$.
3. Find the discrete numerical solution $u_j^h = \mathcal{S}^h(f_j^h, \theta_j^h, \eta_j^h)$.
4. Choose output nodes $\{\boldsymbol{x}_l\}_{l=1}^{L}$ to sample the numerical solution $u_{jl}^h = u_j^h(\boldsymbol{x}_l)$.
5. Generate the input vectors $(\widehat{\boldsymbol{F}}_j, \widehat{\boldsymbol{\Theta}}_j, \widehat{\boldsymbol{N}}_j)$.
6. Collect input & output to form training set with $J \times L$ samples

$$\mathbb{S} = \{(\widehat{\boldsymbol{F}}_j, \widehat{\boldsymbol{\Theta}}_j, \widehat{\boldsymbol{N}}_j, \boldsymbol{x}_l, u_{jl}^h) : 1 \leq j \leq J,\ 1 \leq l \leq L\},$$

Find the network weights that minimize the loss function

$$\Pi(\boldsymbol{\psi}) = \frac{1}{J} \sum_{j=1}^{J} \Pi_j(\boldsymbol{\psi}), \qquad \Pi_j(\boldsymbol{\psi}) = \sum_{l=1}^{L} w_l \left(u_{jl}^h - \widehat{\mathcal{S}}_{\boldsymbol{\psi}}(\widehat{\boldsymbol{F}}_j, \widehat{\boldsymbol{\Theta}}_j, \widehat{\boldsymbol{N}}_j)[\boldsymbol{x}_l] \right)^2.$$

where ψ are all the trainable parameters of the VarMiON.

The generalization error for any $(f, \theta, \eta) \in \mathcal{X}$

$$\mathcal{E}(f, \theta, \eta) := \|\mathcal{S}(f, \theta, \eta) - \widehat{\mathcal{S}}(\widehat{\boldsymbol{F}}, \widehat{\boldsymbol{\Theta}}, \widehat{\boldsymbol{N}})\|_{L^2}.$$

Split into four errors:

$$\begin{aligned}
\mathcal{E}(f, \theta, \eta) \quad \leq \quad & \|\mathcal{S}(f, \theta, \eta) - \mathcal{S}(f_j, \theta_j, \eta_j)\|_{L^2} \longrightarrow \text{Stability of } \mathcal{S} \\
& + \|\mathcal{S}(f_j, \theta_j, \eta_j) - \mathcal{S}^h(f_j^h, \theta_j^h, \eta_j^h)\|_{L^2} \longrightarrow \text{Numerical error in generating data} \\
& + \|\mathcal{S}^h(f_j^h, \theta_j^h, \eta_j^h) - \widehat{\mathcal{S}}(\widehat{\boldsymbol{F}}_j, \widehat{\boldsymbol{\Theta}}_j, \widehat{\boldsymbol{N}}_j)\|_{L^2} \longrightarrow \text{Training error of VarMiON} \\
& + \|\widehat{\mathcal{S}}(\widehat{\boldsymbol{F}}_j, \widehat{\boldsymbol{\Theta}}_j, \widehat{\boldsymbol{N}}_j) - \widehat{\mathcal{S}}(\widehat{\boldsymbol{F}}, \widehat{\boldsymbol{\Theta}}, \widehat{\boldsymbol{N}})\|_{L^2} \longrightarrow \text{Stability of VarMiON } \widehat{\mathcal{S}}
\end{aligned}$$

Generalization error estimate (Patel et al., 2022)

If $\mathcal{X} := \mathcal{F} \times \mathcal{T} \times \mathcal{N}$ is compact, the non-linear branch is Lipschitz, i.e.,

$$\|\boldsymbol{D}(\widehat{\boldsymbol{\Theta}}) - \boldsymbol{D}(\widehat{\boldsymbol{\Theta}}')\|_2 \leq L_D \|\widehat{\boldsymbol{\Theta}} - \widehat{\boldsymbol{\Theta}}'\|_2.$$

Then, the generalization error can be bounded as

$$\mathcal{E}(f, \theta, \eta) \leq \mathcal{C} \left(\epsilon_h + \epsilon_s + \sqrt{\epsilon_t} + \frac{1}{k^{\alpha/2}} + \frac{1}{(k')^{\alpha'/2}} + \frac{1}{L^{\gamma/2}} \right)$$

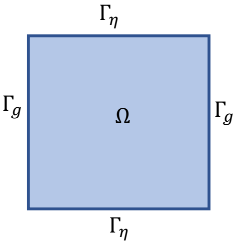
where

$$\begin{aligned} \epsilon_h &\rightarrow \text{numerical error in training data} \\ \epsilon_s &\rightarrow \text{covering estimate} \\ \epsilon_t &\rightarrow \text{training error} \\ \alpha, \alpha', \gamma &\rightarrow \text{quadrature convergence rates} \end{aligned}$$

The constant C depends on the stability constants of $\mathcal{S}$ and $\widehat{\mathcal{S}}$.

Steady-state heat conduction

$$
\begin{aligned}
-\nabla \cdot (\theta(\boldsymbol{x})\nabla u(\boldsymbol{x})) &= f(\boldsymbol{x}), &\quad \forall\, \boldsymbol{x} \in \Omega,\\
\theta(\boldsymbol{x})\nabla u(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) &= \eta(\boldsymbol{x}), &\quad \forall\, \boldsymbol{x} \in \Gamma_\eta,\\
u(\boldsymbol{x}) &= 0, &\quad \forall\, \boldsymbol{x} \in \Gamma_g.
\end{aligned}
$$

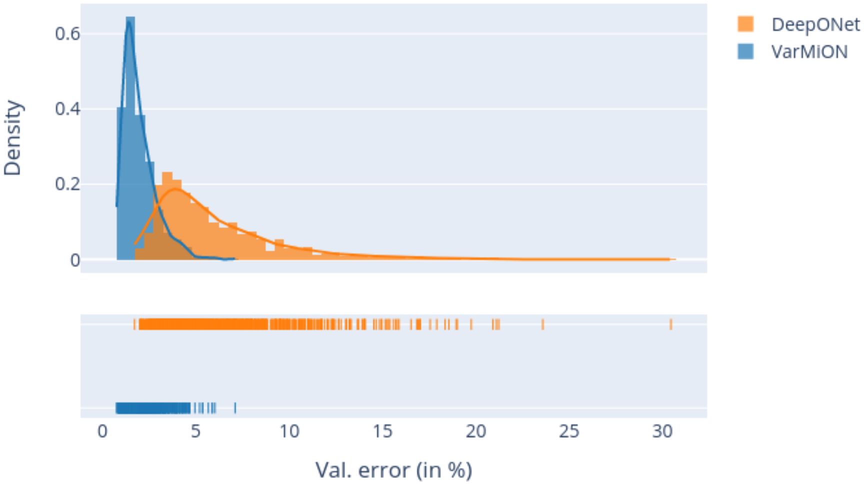


- Input: thermal conductivity θ, heat sources f, and heat flux η. Output: temperature u.
- Inputs: Gaussian Random Fields.
- Networks with two inputs (θ, f) and three inputs (θ, f, η).
- Compare VarMiON ($p = 100$) and vanilla DeepONet.
- Similar number of network parameters. Identical trunk architecture.
- Robustness: sampling (spatially uniform or random) and trunk functions (ReLU or RBF).

- 10,000 samples generated using Fenics.
- 9,000 for training/validation and 1,000 for testing.
- Average value of relative L_2 error reported below.

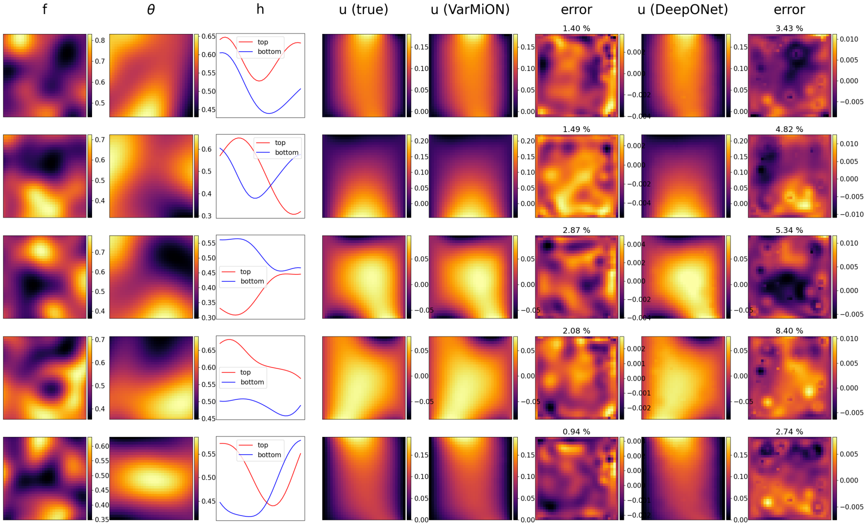
Case	Model	Number of parameters	Relative L_2 error
Two input functions with randomly sampled input	DeepONet (w/ ReLU trunk) VarMiON(w/ ReLU trunk)	111,248 109,013	1.07 ± 0.39 % **0.93** $\pm$ **0.28 %**
Two input functions with uniformly sampled input	DeepONet (w/ ReLU trunk) VarMiON(w/ ReLU trunk)	49,928 46,281	1.98 ± 0.79 % **1.05** $\pm$ **0.42 %**
Two input functions with uniformly sampled input	DeepONet (w/ RBF trunk) VarMiON(w/ RBF trunk)	17,911 17,345	1.39 ± 0.60 % **0.64** $\pm$ **0.35 %**
Three input functions with uniformly sampled input	DeepONet (w/ RBF trunk) VarMiON(w/ RBF trunk)	24,543 23,065	5.99 ± 4.24 % **2.06** $\pm$ **0.90 %**

Density of scaled L_2 error (RBF trunk and uniform spatial sampling).



Numerical Example: Three inputs

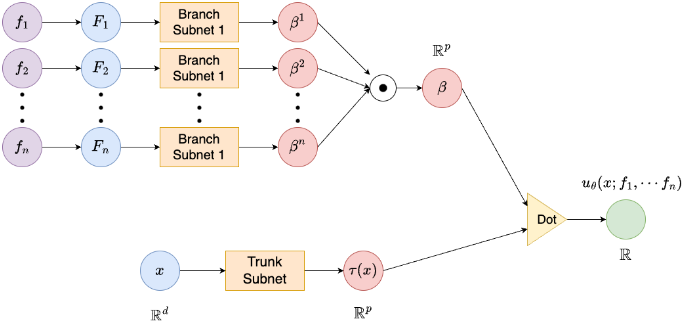
Predictions by VarMiON and DeepONet.



MIONet has been proposed [Jin et al., 2022] to handle multiple input functions.

Separate branch for each f_i, followed by a Hadamard product

$$\beta = (\beta^1 \odot \beta^2 \odot \cdots \odot \beta^n), \quad u_\theta(x; f_1, \cdots, f_n) = \beta^\top \tau(x)$$



Comparison with MIONet as the number of training samples n is varied

Training dataset size	Model	Relative L_2 error
$n = 1000$	DeepONet	10.23 ± 5.20
	MIONet	88.07 ± 69.68
	VarMiON	$\mathbf{4.27 \pm 2.23}$
$n = 2000$	DeepONet	9.00 ± 5.63
	MIONet	85.03 ± 123.77
	VarMiON	$\mathbf{4.04 \pm 1.86}$
$n = 4000$	DeepONet	7.19 ± 3.75
	MIONet	88.39 ± 62.10
	VarMiON	$\mathbf{2.90 \pm 1.50}$
$n = 6000$	DeepONet	6.28 ± 3.55
	MIONet	82.89 ± 34.19
	VarMiON	$\mathbf{2.74 \pm 1.31}$

A word on non-linear PDEs

- VarMiON needs to be carefully constructed due to the dependence on the structure of the variational form.
- Have constructed a VarMiON for the regularized Eikonal equation.
- We believe the VarMiON architecture needs to be customized depending on the type of PDE (ongoing work)

Concluding remarks

- VarMiON: an operator network that mimics variational formulation.
- Takes the form of a reduced order model.
- Precise specification of the branch network – depends on weak form of PDE.
- Error analysis reveals important components – currently investigating training with appropriate Sobolev loss.
- Numerical results point to better and more robust performance.
- Several extensions: other nonlinear operators, physics-informed residuals, time-dependent problems, hyperbolic systems, and specification of geometry.