

Hybrid AI : Variational Data assimilation and operator learning WCCM 2024

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① Hybrid AI

PBDW Intro

PBDW Algebraic formulation

Deeponets

Soft Constrain

Hard Constrain

② Numerical Result - Helmholtz Equation

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Parameterized-Background Data-Weak (PBDW) (A Patera, Y Maday, J Penn and MYano)

The idea is to look for the state u_{true} of a parameterized model as a sum of contributions.

$$u_{N,M} = z_{N,M} + \eta_{N,M} = \Pi_{Z_N} u^{\text{true}} + \Pi_{Z_N^\perp} u^{\text{true}} \quad (1)$$

- u not lying on the background manifold, motivates the second contribution $\eta_{N,M}$.

Offline - Background and Observable Space

- $\mathcal{Z}_N = \text{span} \{ \zeta_n \}_{n=1}^N \subset \mathcal{U}$ is a N -dimensional space that represents \mathcal{M}^{bk} .
- $\mathcal{U}_M = \text{span} \{ q_m \equiv R_{\mathcal{U}} \ell_m^o \}_{m=1}^M$, $M = 1, \dots, M_{\max}, \dots$

With $R_{\mathcal{U}} \ell \in \mathcal{U}$ the Riesz representation of $\ell \in \mathcal{U}'$

$$(u^{\text{true}}, q_m) = (u^{\text{true}}, R_{\mathcal{U}} \ell_m^o) = \ell_m^o(u^{\text{true}})$$

The state is given by $u_{N,M}^* = z_{N,M}^* + \eta_{N,M}^* = \sum_{n=1}^N \zeta_n z_n^* + \sum_{m=1}^M q_m \eta_m^*$

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Limited and homoscedastic noisy observations PBDW

Find $(z_{N,M}^\xi, \eta_{N,M}^\xi) \in \mathcal{Z}_N \times \mathcal{U}_M$ such that:

$$(z_{N,M}^\xi, \eta_{N,M}^\xi) = \arg \inf_{\substack{z \in \mathcal{Z}_N \\ \eta \in \mathcal{U}_M}} \left(\xi \|\eta\|^2 + \frac{1}{M} \sum_{m=1}^M \|l_m(z + \eta) - y_m\|_2^2 \right) \quad (3)$$

$\|\cdot\|_2$ the Euclidean L^2 -norm in \mathbb{R}^M

ξ the regularization tuning the approximation between \mathcal{Z}_N and \mathcal{U}_M .

Online - Algebraic formulation

- $A_{mm'} = (q_{m'}, q_m) \in \mathbb{R}^{M_{\max} \times M_{\max}}, \quad m, m' = 1, \dots, M_{\max}$
- $B_{mn} = (\zeta_n, q_m) \in \mathbb{R}^{M_{\max} \times N_{\max}}, \quad m = 1, \dots, M_{\max}, n = 1, \dots, N_{\max}$

$$\begin{bmatrix} \xi M \mathbb{I}_M + \mathbb{A} & \mathbb{B} \\ \mathbb{B}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\eta}^* \\ \mathbf{z}^* \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ 0 \end{bmatrix} \quad (4)$$

Orthogonality property

From the equation $(4)_2$:

$$\mathbb{B}^T \boldsymbol{\eta}^* = 0 \iff (\boldsymbol{\eta}^*, \boldsymbol{z}) = 0 \quad \forall \boldsymbol{z} \in \mathcal{Z}_N \quad (5)$$

Naturally leading to

$$\boldsymbol{\eta}_{N,M}^* \in \mathcal{U}_M \cap \mathcal{Z}_N^\perp \quad (6)$$

Sensors Selection : Stability-Approximation

$$\text{Unique solution if } \beta_{N,M} = \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{U}_M} \frac{((z, q))}{\|z\| \|b\|} > 0$$

(7)

2 steps :

- maximize the inf-sup(stability) constant $\beta_{N,M}$;
- minimize the background best-fit error $\epsilon_N^{bk} = \inf_{z \in \mathcal{Z}_N} \|u_{\text{true}} - z\| = \left\| \Pi_{\mathcal{Z}_N^\perp} u_{\text{true}} \right\|$

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Universal Approximation Theorem for Operator (L Lu, P Jin, G Pang, Z Zhang G Karniadakis)

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

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

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Soft Constrain Architecture

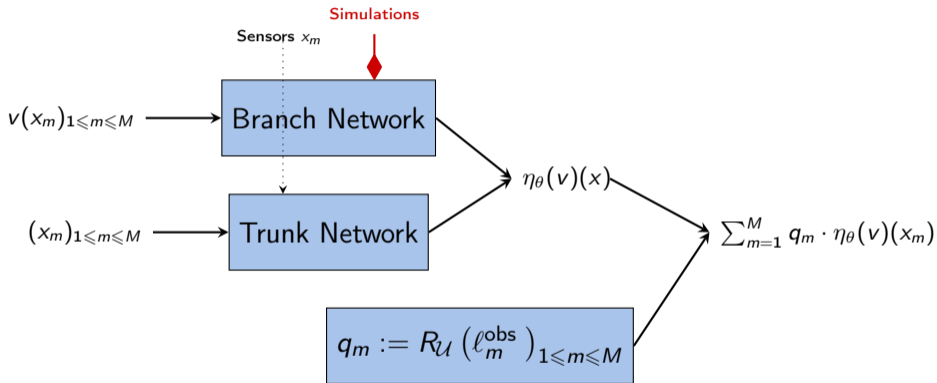


Figure 1: DeepONet with weak orthogonality

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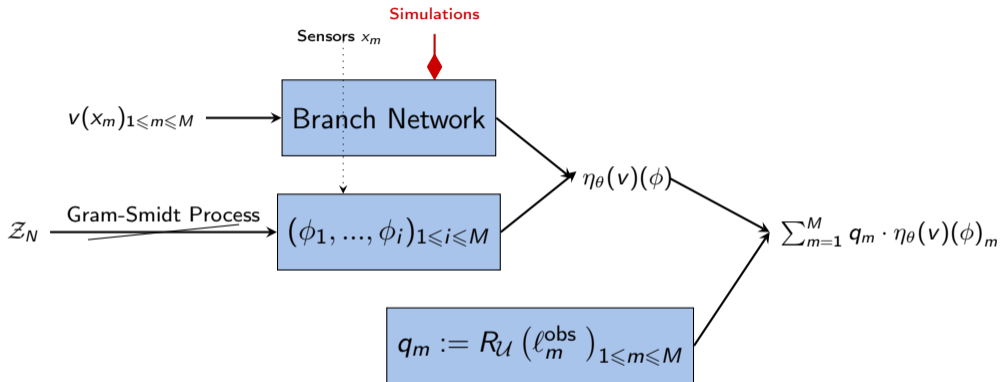


Figure 2: DeepONet with strong orthogonality

$$\begin{aligned}\langle \eta_\theta(v)(\phi), \zeta_n \rangle &= \eta_{\theta N+1} \langle \phi_{N+1}, \zeta_n \rangle + \eta_{\theta N+2} \langle \phi_{N+2}, \zeta_n \rangle + \dots + \eta_{\theta M-N} \langle \phi_M, \zeta_n \rangle \\ &= 0 + 0 + \dots + 0\end{aligned}$$

$\eta_\theta(v)(\phi)$ lies in $\mathcal{U}_M \cap \mathcal{Z}_N^\perp$ by construction. Thus accommodates the part of the projection onto \mathcal{U}_M which cannot be absorbed by $z_{N,M}^* \in \mathcal{Z}_N$.

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② Numerical Result - Helmholtz Equation

2D Helmholtz equation in a homogeneous medium $\Omega = [0; 1]^2$, $\epsilon = 0.01$

$$\begin{cases} -(1 + \epsilon\mu i)\Delta u(x) - \mu^2 u(x) = \mu q & \forall x \in \mathbb{R}^2 \cap \Omega. \\ \mathcal{B}(u)(x) & \forall x \in \mathbb{R}^2 \cap \partial\Omega \end{cases} \quad (8)$$

q the source defined on Ω :

$$q(x_1, x_2) = \sin(\mu x_1) * \sin(\mu x_2) + g \quad (9)$$

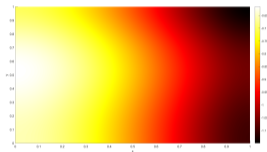
g the bias associated to the modeling of q .

$$g(x_1, x_2) := \begin{cases} 0 & \text{(perfect source)} \\ -0.5 (\sin(e^{-3x_1} * \sin(5\mu x_2))) & \text{(wrong source)} \end{cases} \quad (10)$$

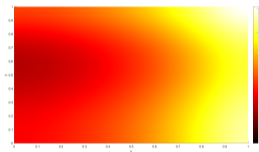
$\mathcal{B}(u)$ the boundary conditions operator.

$$\mathcal{B}(u) := \begin{cases} u(x) = 0 & \forall x \in \mathbb{R}^2 \cap \partial\Omega & \text{(wrong boundary condition)} \\ \partial_n u(x) = 0 & \forall x \in \mathbb{R}^2 \cap \partial\Omega & \text{(perfect boundary condition)} \end{cases} \quad (11)$$

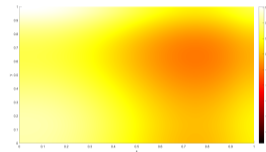
Background Space



(a) ζ_1



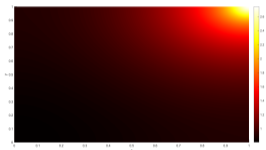
(b) ζ_2



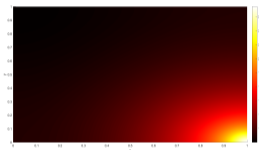
(c) ζ_3

Figure 3: $\mathcal{Z}_N = \text{span} \{ \zeta_n \}_{1 \leq n \leq N}$

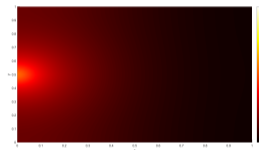
Observation Space



(a) $R_{\mathcal{U}}(\ell_1^{\text{obs}})$



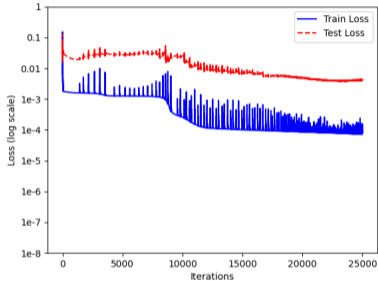
(b) $R_{\mathcal{U}}(\ell_2^{\text{obs}})$



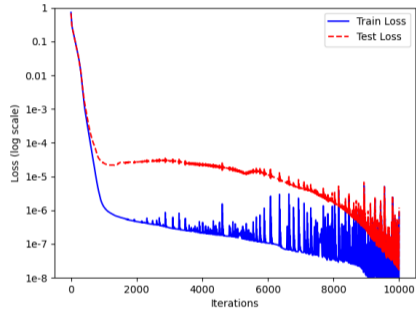
(c) $R_{\mathcal{U}}(\ell_3^{\text{obs}})$

Figure 4: $\mathcal{U}_M := \text{Span}\{q_m\}_{1 \leq m \leq M}$

Loss evolution



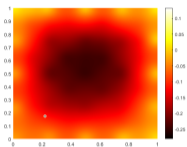
(a) Physics Inspired



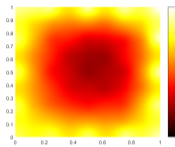
(b) Physics Constrained

Figure 5: Orthogonality Constraint

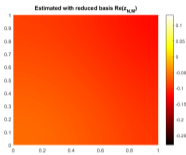
Wrong Source



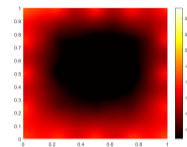
(a) Prediction of $\eta_{2,50}$



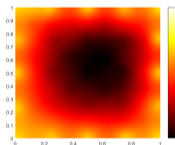
(b) PBDW $\eta_{2,50}$



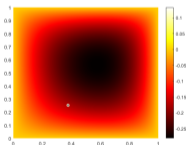
(c) PBDW $z_{2,50}$



(d) Hybrid twin $u_{2,50}$

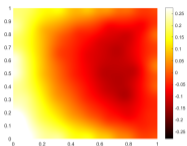


(e) PBDW $u_{2,50}$

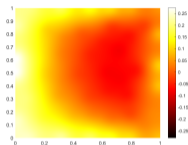


(f) Ground Truth

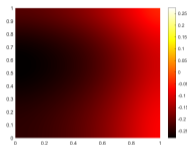
Wrong Source - Wrong Boundaries conditions



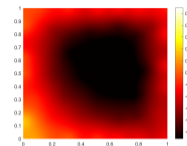
(a) Prediction of $\eta_{2,50}$



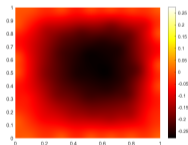
(b) PBDW $\eta_{2,50}$



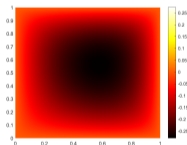
(c) PBDW $z_{2,50}$



(d) Hybrid twin $u_{2,50}$

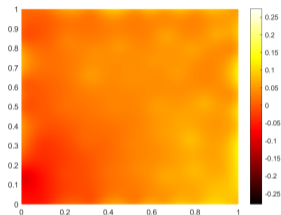


(e) PBDW $u_{2,50}$

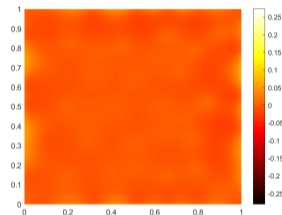


(f) Ground Truth

Error Map



(a) Hybrid Twin



(b) PBDW

Figure 8: $RelativeL_2(\Omega)$ error