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Hybrid AI : Biais-Aware Data Assimilation with Operator Learning

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Reality = Knowledge + Ignorance

Challenge: Optimal recovery of an element of a Hilbert space $u \in \mathcal{U}$ from measurements $\ell_m^{\text{obs}}\left(u^{\text{true}}\right)$ leads to suboptimal recovery when u is governed by a biased model $\mathcal{P}(u, \mu)$. We want to estimate the state u^{true} while being aware of the model bias(unanticipated physics).

Key idea: We integrate a Deep Neural Operators (Deeponet) in the Parameterized Background Data-Weak (PBDW) to accommodate the deficient physics.

PBDW Formulation

Given M measurements $\ell_m^{\text{obs}}\left(u^{\text{true}}\right)$ and a parametric model $\mathcal{P}(u, \mu)$. For a given parameter value μ, PBDW estimate the state as a combination of 2 contributions

$u_{N,M} = z_{N,M} + \eta_{N,M} = \Pi_{\mathcal{Z}_N} u^{\text{true}} + \Pi_{\mathcal{U}_M \cap \mathcal{Z}_N^{\perp}} u^{\text{true}}$

such that :

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

The first contribution z represent the anticipated uncertainty. The second constribution η , called update represent the unanticipated physics. We want to learn the update with a neural operator.

Construction of Spaces : Offline

- **Background Space** $\mathcal{Z}_N := \operatorname{span}\{\zeta_n\}_{n=1}^{N}$
  - ∗ Reduced model N-dimensional linear space of a high dimensional parametric manifold $\mathcal{M}^{\text{bk}} = \{u(\mu) \mid \mu \in \mathcal{D}\}$
  - ∗ Minimize background best-fit error $\inf_{z \in \mathcal{Z}_N} \|u^{\text{true}} - z\|$
- **Experimentally Observable Space** $\mathcal{U}_M := \operatorname{span}\{q_m\}_{m=1}^{M}$
  - ∗ q_m Riesz representation of $\ell_m^{\text{obs}} / (u^{\text{true}}, q_m) = \ell_m^{\text{obs}}\left(u^{\text{true}}\right)$.
  - ∗ Maximize stability $\beta_{N,M} = \inf_{z \in \mathcal{Z}_N} \sup_{q \in \mathcal{U}_M} \frac{((z,q))}{\|z\|\|b\|}$.
  - ∗ Minimize Approx error $\inf_{\eta \in \mathcal{U}_M \cap \mathcal{Z}_N^{\perp}} \left\| \Pi_{\mathcal{Z}_N^{\perp}} u^{\text{true}} - \eta \right\|$.

Bias-Operator

We parameterize the update η with a Deeponets $\eta_\theta(v)(x_m)$ constrained to lie in $\mathcal{U}_M \cap \mathcal{Z}_N^{\perp}$

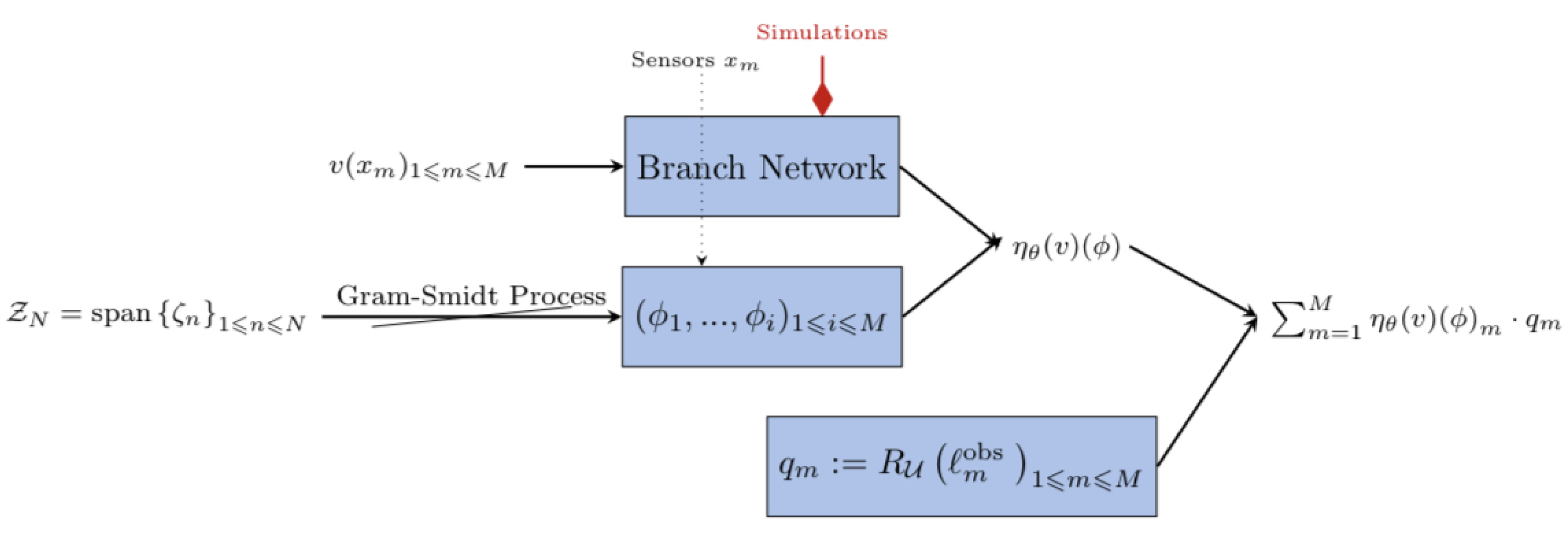


Figure 1: Deeponets with orthogonality constrain

Algebraic formulation

The problem reads: find $(z_{N,M}, \eta_\theta) \in \mathcal{Z}_N \times \mathcal{U}_M$ such that

$$\begin{cases} (\eta_\theta, q) + (z_{N,M}, q) = (u^*, q), \quad \forall q \in \mathcal{U}_M, \\ (\eta_\theta, p) = 0, \quad \forall p \in \mathcal{Z}_N, \\ \theta^* = \arg\min_\theta \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} \left[\sum_{j=1}^{M} \hat{\eta}_j(y_i; \theta) \cdot \phi_j - \eta^*(y_i) \right]^2. \end{cases}$$

In algebraic form, the Operator-PBDW statement reads:
find $(\boldsymbol{z}_{N,M}, \boldsymbol{\eta_\theta}) \in \mathbb{R}^N \times \mathbb{R}^M$ such that

$$\begin{bmatrix} \xi M \mathbb{I}_M + \mathbb{A} & \mathbb{B} \\ \mathbb{B}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\eta_\theta}^\star \\ \mathbf{z}^\star \end{bmatrix} = \begin{bmatrix} \boldsymbol{y} \\ \mathbf{0} \end{bmatrix}$$

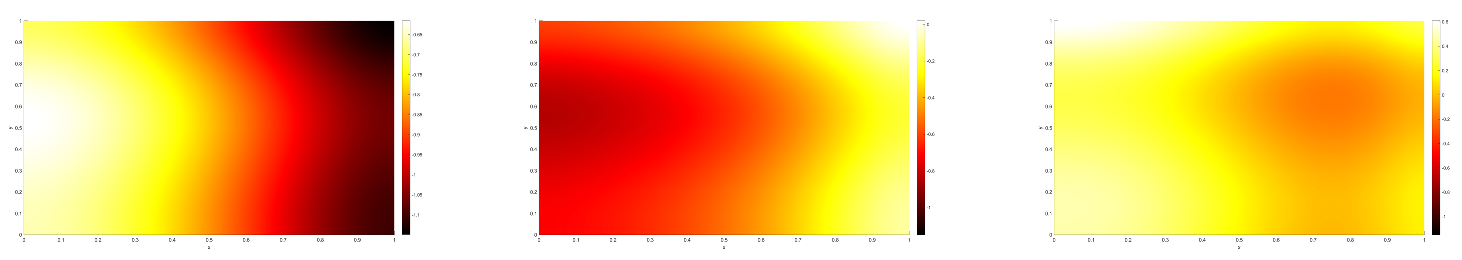
Given the matrix $\mathbf{A}_{mm'} = (q_{m'}, q_m), \mathbf{B}_{mn} = (\zeta_n, q_m)$

The neural operator lies in $\mathcal{U}_M \cap \mathcal{Z}_N^{\perp}$ leading to $\mathbb{B}^T \cdot \boldsymbol{\eta_\theta}^\star = 0$, hence accomodate strictly unanticipated physics.

Experiments - 2D Helmoltz Equation

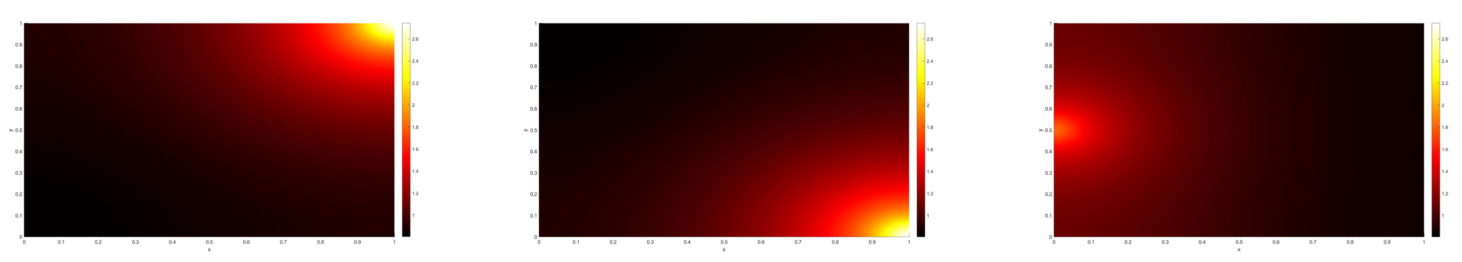
$$\begin{cases} -(1 + \epsilon\mu i)\Delta u(x) - \mu^2 u(x) = \mu\, q\, \forall x \in \mathbb{R}^2 \cap \Omega. \\ \mathcal{B}(u)(x)\, \forall x \in \mathbb{R}^2 \cap \partial\Omega \end{cases} \tag{2}$$

q the sourcing term and $B(u)$ the boundary conditions operator.



(a) ζ_1 (b) ζ_2 (c) ζ_3

Figure 2: Backgound POD Modes



(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 3: Riezs Representers

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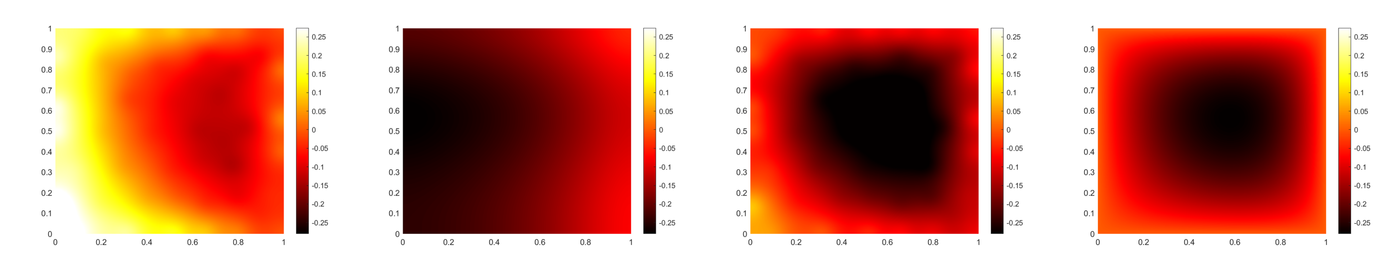
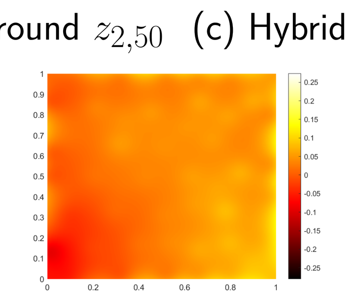


(a) Prediction of $\eta_{2,50}$ (b) Background $z_{2,50}$ (c) Hybrid twin $u_{2,50}$ (d) Ground Truth



(e) Rel. $L_2(\Omega)$ Error

Figure 4: Bias from source & Boundary Conditions

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