An Adaptive PBDW approach to state estimation

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Acknowledgments: Y Maday (UPMC, Brown), and AT Patera (MIT).

Formulation

Data assimilation: state estimation

Given a physical system, we wish to integrate

a *best-knowledge* model with uncertain parameters,

and M experimental observations

to estimate the state u^{true} over the domain $\Omega \subset \mathbb{R}^d$.

Data assimilation: state estimation

Given a physical system, we wish to integrate

a *best-knowledge* model with uncertain parameters,

$G^{\mathrm{bk},\mu}(u^{\mathrm{bk}}(\mu)) = 0,$

$\mu \in \mathcal{P}^{\mathrm{bk}}$ uncertain model parameters,

well-posed over $\Omega^{\mathrm{bk}} \supset \Omega$,

and M experimental observations

$y_m = \ell_m^o(u^{\mathrm{true}}) + \epsilon_m,\ m = 1, \ldots, M$

$\ell_1^o, \ldots, \ell_M^o$ linear functionals,

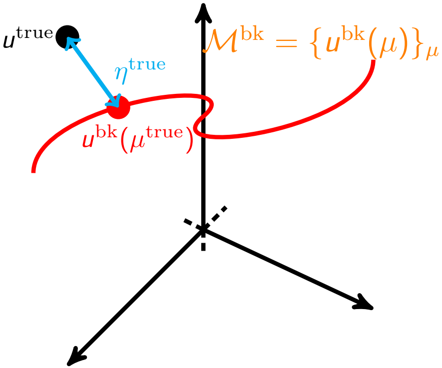
$\mathcal{L}_M = [\ell_1^o, \ldots, \ell_M^o]$,

to estimate the state u^{true} over the domain $\Omega \subset \mathbb{R}^d$.

Decomposition of the true field

Given the functional space $\mathcal{U}$, write $u^{\rm true}$ as

$$u^{\rm true} = u^{\rm bk}(\mu^{\rm true}) + \eta^{\rm true},\ \mu^{\rm true} \in \mathcal{P}^{\rm bk},\ \eta^{\rm true} \in \mathcal{U}.$$



$\mu^{\rm true} :=$

$$\arg\min_\mu \| u^{\rm true} - u^{\rm bk}(\mu) \|$$

addresses uncertainty in μ

$\eta^{\rm true} := u^{\rm true} - u^{\rm bk}(\mu^{\rm true})$

addresses model uncertainty

Estimate $(\mu^{\text{true}}, \eta^{\text{true}})$: Partial Spline Model (Wahba, 1990)

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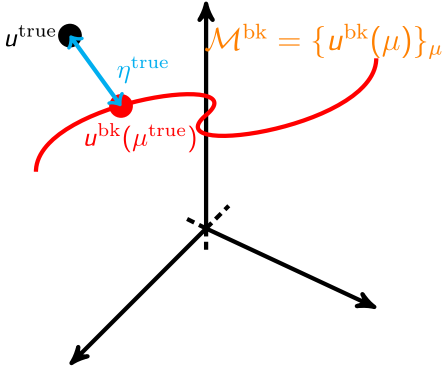
$$\eta^{\text{true}} := u^{\text{true}} - u^{\text{bk}}(\mu^{\text{true}})$$

addresses model uncertainty



PSM: $$\min_{(\mu,\eta)\in\mathcal{P}^{\text{bk}}\times\mathcal{U}} \underbrace{\xi\|\eta\|^2}_{\text{penalty}} + \underbrace{V_M\left(\mathcal{L}_M(u^{\text{bk}}(\mu)+\eta) - \mathbf{y}\right)}_{\text{data misfit}}$$

Reformulation of the PSM: rank-N approximations

Substitute $u^{\mathrm{bk}}(\mu)$ with the rank-N approximation:

$$u_N^{\mathrm{bk}}(x,\mu) := \sum_{n=1}^{N} \alpha_n(\mu)\zeta_n(x), \quad \mu \in \mathcal{P}^{\mathrm{bk}}, \;\; x \in \Omega \subset \Omega^{\mathrm{bk}}.$$

$$\min_{(\mu,\eta)\in\mathcal{P}^{\mathrm{bk}}\times\mathcal{U}} \xi\|\eta\|^2 + V_M\left(\mathcal{L}_M\left(\sum_{n=1}^{N}\alpha_n(\mu)\zeta_n + \eta\right) - \mathbf{y}\right)$$

state estimate: $u_\xi^\star = \sum_{n=1}^{N}\alpha_n(\mu_\xi^\star)\zeta_n + \eta_\xi^\star.$

Reformulation of the PSM: rank-N approximations

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Define $\Phi_N := \{[\alpha_1(\mu), \ldots, \alpha_N(\mu)] : \; \mu \in \mathcal{P}^{\mathrm{bk}}\} \subset \mathbb{R}^N$.

Minimize over $(\boldsymbol{\alpha}, \eta) \in \Phi_N \times \mathbb{R}^N$

$$\min_{(\boldsymbol{\alpha},\eta)\in\Phi_N\times\mathcal{U}} \xi\|\eta\|^2 + V_M\left(\mathcal{L}_M\left(\sum_{n=1}^{N}\alpha_n\zeta_n + \eta\right) - \mathbf{y}\right)$$

state estimate: $$u_\xi^\star = \sum_{n=1}^{N} \alpha_{\xi,n}^\star \zeta_n + \eta_\xi^\star.$$

Introduce the approximation of Φ_N, $\widetilde{\Phi}_N \subset \mathbb{R}^N$.

Then, obtain the **PBDW statement**:

$$\min_{(\boldsymbol{\alpha},\eta)\in\widetilde{\Phi}_N\times\mathcal{U}} \xi\|\eta\|^2 + V_M\left(\mathcal{L}_M\left(\sum_{n=1}^{N}\alpha_n\zeta_n + \eta\right) - \mathbf{y}\right)$$

Relaxation: PSM $\to$ PBDW

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The Partial Spline Model is non-convex, and highly nonlinear.

If $\widetilde{\Phi}_N$ is convex, the PBDW statement is a convex relaxation of the PSM.

If $\widetilde{\Phi}_N$ is a convex polytope and $V_M(\mathbf{w}) = \mathbf{w}^T\mathbb{O}\mathbf{w}$, the PBDW statement is a QP.

PSM $\rightarrow$ PBDW: the role of MOR

PBDW relies on a N-term approximation of u^{bk}:

$$u^{\mathrm{bk}}(x,\mu) \approx \sum_{n=1}^{N} \alpha_n(\mu)\,\zeta_n(x) \quad \forall\, \mu \in \mathcal{P}^{\mathrm{bk}},\; x \in \Omega,$$

where $N \leq M$ due to stability issues.

MOR provides efficient tools for **data compression**.

PSM $\to$ PBDW: the role of MOR

PBDW relies on a N-term approximation of $u^{\rm bk}$:

$$u^{\rm bk}(x,\mu) \approx \sum_{n=1}^{N} \alpha_n(\mu)\,\zeta_n(x) \quad \forall\,\mu \in \mathcal{P}^{\rm bk},\; x \in \Omega,$$

where $N \le M$ due to stability issues.

MOR provides efficient tools for **data compression**.

Data compression: given the *bk manifold*

$$\mathcal{M}^{\rm bk} = \{u^{\rm bk}(\mu)|_{\Omega} : G^{{\rm bk},\mu}(u^{\rm bk}(\mu)) = 0,\ \mu \in \mathcal{P}^{\rm bk}\}$$

find a *background* space $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^{N}$ s.t.

$$\sup_{\mu \in \mathcal{P}^{\rm bk}} \inf_{z \in \mathcal{Z}_N} \| u^{\rm bk}(\mu)|_{\Omega} - z \| \text{ is small.}$$

PBDW formulation: contribution and challenges

General formulation:

$$\min_{(\boldsymbol{\alpha},\eta)\in\widetilde{\Phi}_N\times\mathcal{U}} \xi\|\eta\|^2 + V_M\left(\mathcal{L}_M\left(\sum_{n=1}^{N}\alpha_n\zeta_n+\eta\right)-\mathbf{y}\right)$$

Main features

Two-level mechanism to accomodate parametric and non-parametric model uncertainty.

Use of MOR to generate a linear surrogate $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^N$ of $\mathcal{M}^{\mathrm{bk}} = \{u^{\mathrm{bk}}(\mu')|_\Omega : \mu' \in \mathcal{P}^{\mathrm{bk}}\}$.

PBDW formulation: contribution and challenges

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$$\min_{(\boldsymbol{\alpha},\eta)\in\widetilde{\Phi}_N\times\mathcal{U}} \xi\|\eta\|^2 + V_M\left(\mathcal{L}_M\left(\sum_{n=1}^{N}\alpha_n\zeta_n + \eta\right) - \mathbf{y}\right)$$

Challenges and open questions

Choice of $V_M, (\mathcal{U}, \|\cdot\|), \xi$

$\leftrightarrow$ model selection (Machine Learning)

Choice of $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^N$

$\Omega = \Omega^{\mathrm{bk}} \leftrightarrow$ monolithic MOR

$\Omega \subset \Omega^{\mathrm{bk}} \leftrightarrow$ component-based MOR

Choice of $\widetilde{\Phi}_N$.

A few references

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Binev, Cohen, Mula, Nichols, *Greedy algorithms for optimal measurements selection in state estimation using reduced models*, (submitted).

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Agenda of the talk

We consider the formulation

$$\min_{(z,\eta)\in\mathcal{Z}_N\times\mathcal{U}} \xi\|\eta\|^2 + \frac{1}{M}\sum_{m=1}^{M}\left(\ell_m^o(z+\eta)\, -\, y_m\right)^2,$$

which corresponds to $\widetilde{\Phi}_N = \mathbb{R}^N, \;\; V_M = \frac{1}{M}\|\cdot\|_2^2$.

Topics of the talk: choice of $(\mathcal{U}, \|\cdot\|)$;

a priori error analysis;

construction of $\mathcal{Z}_N$ for $\Omega \subset \Omega^{\mathrm{bk}}$.

Hypothesis: $\ell_m^o(z) = 0,\; z \in \mathcal{Z}_N \Leftrightarrow z \equiv 0$

$(\mathcal{Z}_N, \mathcal{L}_M)$ - *unisolvency*

Comparison with a Model-Based (MB) formulation

Given $\mathcal{U}_{\mathrm{bk}} = \mathcal{U}_{\mathrm{bk}}(\Omega^{\mathrm{bk}})$, find $(\mu_\xi^\star, u_\xi^\star)$ s.t.

$$\min_{\substack{\mu\in\mathcal{P}, u\in\mathcal{U}_{\mathrm{bk}} \\ \eta\in\mathcal{U}_{\mathrm{adm}}\subset\mathcal{U}'_{\mathrm{bk}}}} \xi\|\eta\|_\star^2 + V_M(\mathcal{L}_M(u|_\Omega) - \mathbf{y}) \text{ s.t. } \mathcal{G}^{\mathrm{bk},\mu}(u) = \eta,$$

Comparison with a Model-Based (MB) formulation

Given $\mathcal{U}_{\rm bk} = \mathcal{U}_{\rm bk}(\Omega^{\rm bk})$, find $(\mu_\xi^\star, u_\xi^\star)$ s.t.

$$\min_{\substack{\mu\in\mathcal{P}, u\in\mathcal{U}_{\rm bk} \\ \eta\in\mathcal{U}_{\rm adm}\subset\mathcal{U}_{\rm bk}'}} \xi\|\eta\|_\star^2 + V_M(\mathcal{L}_M(u|_\Omega) - \mathbf{y}) \ \text{ s.t. } \ \mathcal{G}^{\rm bk,\mu}(u) = \eta,$$

1. MB is equivalent to PSM for $\mathcal{P} = \{\bar{\mu}\}$, if $\Omega^{\rm bk} = \Omega$, $\mathcal{G}^{\rm bk,\mu}(\cdot) = \mathcal{A}_\mu(\cdot) - \mathcal{F}_\mu$, and $\|\cdot\|_\star = \|\mathcal{A}_\mu^{-1}(\cdot)\|$; i.e.,
$$u_\xi^\star = \arg\min_{u\in\mathcal{U}} \xi\|u - u^{\rm bk}(\bar{\mu})\|^2 + V_M(\mathcal{L}_M(u) - \mathbf{y})$$
2. MB can prescribe the allowed model biases $\mathcal{U}_{\rm adm}$.
   advantage over PSM/PBDW
3. For $\mathcal{P} \neq \{\bar{\mu}\}$, MB is highly nonlinear, difficult to convexify, and ill-suited to tackle pbs with $\Omega \subsetneq \Omega^{\rm bk}$.
   disadvantage compared to PBDW

Choice of $(\mathcal{U}, \|\cdot\|)$

Choice of $(\mathcal{U}, \|\cdot\|)$: variational update

Choose $\mathcal{U} = \mathcal{X}$, $\|\cdot\| = \|\cdot\|_{\mathcal{X}}$ $\quad (\mathcal{X} = H^1(\Omega), V_{\mathrm{div}}, \dots)$

$$\Rightarrow \eta_\xi^\star \text{ belongs to } \mathcal{U}_M = \mathrm{span}\{R_{\mathcal{X}}\ell_m^o\}_{m=1}^M$$

$$(R_{\mathcal{X}}\ell_m^o, v)_{\mathcal{X}} = \ell_m^o(v) \;\; \forall v \in \mathcal{X}$$

Choice of $(\mathcal{U}, \|\cdot\|)$: variational update

Choose $\mathcal{U} = \mathcal{X}$, $\|\cdot\| = \|\cdot\|_{\mathcal{X}}$ $\quad (\mathcal{X} = H^1(\Omega), V_{\mathrm{div}}, \ldots)$

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$$(R_{\mathcal{X}} \ell_m^o, v)_{\mathcal{X}} = \ell_m^o(v) \;\; \forall v \in \mathcal{X}$$

Originally proposed in [Maday *et al.*, 2015]

The approximation properties of $\mathcal{U}_M$ depend on $\|\cdot\|_{\mathcal{X}}$ and on $\{\ell_m^o\}_{m=1}^M$

Construction of $\mathcal{U}_M$ requires the solution to M Riesz problems.

Choice of $(\mathcal{U}, \|\cdot\|)$: user-defined update

Choose $\mathcal{U} = \mathcal{U}_M = \mathrm{span}\{\psi_m\}_{m=1}^{M} \subset \mathcal{X}$, $\|\cdot\| = \|\cdot\|_{\mathcal{X}}$ s.t.

$\ell_m^o(\psi) = 0, \psi \in \mathcal{U}_M \Leftrightarrow \psi \equiv 0$ ($(\mathcal{U}_M, \mathcal{L}_M)$ - *unisolvency*)

Choice of $(\mathcal{U}, \|\cdot\|)$: user-defined update

Choose $\mathcal{U} = \mathcal{U}_M = \mathrm{span}\{\psi_m\}_{m=1}^M \subset \mathcal{X}$, $\|\cdot\| = \|\cdot\|_{\mathcal{X}}$ s.t.

$\ell_m^o(\psi) = 0, \psi \in \mathcal{U}_M \Leftrightarrow \psi \equiv 0$ ($(\mathcal{U}_M, \mathcal{L}_M)$ - *unisolvency*)

The unisolvency condition guarantees wellposedness.

$\psi_1, \ldots, \psi_M$ are chosen based on approximation considerations.

$\psi_1, \ldots, \psi_M$ *might or might not* depend on the choice of $\|\cdot\|$.

Practical choices of $\psi_1, \ldots, \psi_M$ for local measurements

Given functionals of the form $\ell_m^o = \ell\left(\cdot, x_m^o, r_{\mathrm{w}}\right)$,

$$\ell\left(v, \bar{x}, r_{\mathrm{w}}\right) = C(r_{\mathrm{w}}) \int_\Omega \omega\left(\frac{\|x - \bar{x}\|_2}{r_{\mathrm{w}}}\right) v(x)\, dx,$$

$\ell_m^o \to \delta_{x_m^o}$ for $r_{\mathrm{w}} \to 0^+$

possible choices are

1. $\psi_m(\cdot) = \Phi\left(\|\cdot - x_m^o\|_2\right)$ where Φ is a PD RBF, or

   no need for solving M offline Riesz problems,

2. $\psi_m(\cdot) = R_{\mathcal{X}} \ell\left(\cdot, x_m^o, R_{\mathrm{w}}\right)$ where $R_{\mathrm{w}} > r_{\mathrm{w}}$.

   simple treatment of strong BCs

Equivalence between variational and user-defined updates

Define $\mathcal{I}_M : \mathcal{X} \to \mathcal{U}_M$ s.t. $\mathcal{L}_M(\mathcal{I}_M(v)) = \mathcal{L}_M(v) \ \forall v \in \mathcal{X}$

Proposition: let $\mathcal{U}_M = \mathrm{span}\{\psi_m\}_m$ satisfy unisolvency condition. Then, PBDW solution solves:

$$\min_{(z,\eta)\in\mathcal{Z}_N\times\mathcal{X}} \xi|||\eta|||^2 + V_M(\mathcal{L}(z+\eta) - \mathbf{y})$$

where $|||u|||^2 = \|\mathcal{I}_M(u)\|_{\mathcal{X}}^2 + \|u - \mathcal{I}_M(u)\|_{\mathcal{X}}^2$ is an equivalent norm for $\mathcal{X}$.

Variational approach: choose $(\mathcal{X}, \|\cdot\|_{\mathcal{X}}) \Rightarrow \mathcal{U}_M$;

User-defined approach: choose $\mathcal{U}_M \Rightarrow (\mathcal{X}, |||\cdot|||)$.

link with kernel methods for regression

A priori error analysis

Preliminaries

Suppose $y_m = \ell_m^o(u^{\mathrm{true}}) + \epsilon_m, \quad m = 1, \ldots, M$, where $\epsilon_m \overset{\mathrm{iid}}{\sim} (0, \sigma^2)$ (*homoscedastic noise*).

Introduce $u_{\xi=0}^{\mathrm{opt}}$ PBDW solution for $\xi \to 0^+$ fed with perfect observations.

Define $(\mathbb{L}_\eta)_{m,m'} = \ell_m^o(\psi_{m'})$, and introduce

$$\mathbf{u} = \left[\begin{array}{c} \boldsymbol{\alpha} \\ \tilde{\boldsymbol{\eta}} = \mathbb{L}_\eta^{-T} \boldsymbol{\eta} \end{array} \right] \leftrightarrow u = \sum_{n=1}^{N} \alpha_n \zeta_n + \sum_{m=1}^{M} \eta_m \psi_m .$$

$$u_\xi^\star \in \mathcal{X} \leftrightarrow \mathbf{u}_\xi^\star \in \mathbb{R}^{N+M},$$
$$u_{\xi=0}^{\mathrm{opt}} \in \mathcal{X} \leftrightarrow \mathbf{u}_{\xi=0}^{\mathrm{opt}} \in \mathbb{R}^{N+M}.$$

Introduce $(\mathbb{L}_\eta)_{m,m'} = \ell^o_m(\psi_{m'})$, and

$$\mathbb{A}(\xi) = \begin{bmatrix} \xi M \mathbb{I} + \mathbb{L}_\eta \mathbb{L}_\eta^T & \mathbb{L}_z \\ \mathbb{L}_z^T & 0 \end{bmatrix} \text{ with } \begin{array}{l} (\mathbb{L}_z)_{m,n} = \ell^o_m(\zeta_n) \\ y_m^{\mathrm{true}} = \ell^o_m(u^{\mathrm{true}}) \end{array},$$

Then, we find

$$\mathbb{A}(\xi)\,\mathbf{u}^\star_\xi = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}, \quad \mathbb{A}(\xi = 0)\,\mathbf{u}^{\mathrm{opt}}_{\xi=0} = \begin{bmatrix} \mathbf{y}^{\mathrm{true}} \\ \mathbf{0} \end{bmatrix}$$

Error analysis for perfect measurements

Introduce

the inf-sup constant $\beta_{N,M} = \inf_{z \in \mathcal{Z}_N} \sup_{v \in \mathcal{U}_M} \dfrac{((z,v))}{|||z|||\,|||v|||}$, and

the Lebesgue constant $\|\mathcal{I}_M\|_{\mathcal{L}(\mathcal{X})} = \sup_{v \in \mathcal{X}} \dfrac{\|\mathcal{I}_M(v)\|_{\mathcal{X}}}{\|v\|_{\mathcal{X}}}$.

$(= 1 \text{ for } \mathcal{U}_M = \mathrm{span}\{R_{\mathcal{X}} \ell_m^o\}_m)$

Then,

$$\|u^{\rm true} - u^{\rm opt}_{\xi=0}\|_{\mathcal{X}} \leq \frac{\sqrt{4 + 6\|\mathcal{I}_M\|^2_{\mathcal{L}(\mathcal{X})}}}{\beta_{N,M}} \times \inf_{z \in \mathcal{Z}_N} \inf_{q \in \mathcal{U}_M \cap \mathcal{Z}_N^{\perp, |||\cdot|||}} \|u^{\rm true} - z - q\|_{\mathcal{X}}.$$

Error analysis for imperfect measurements

Bias: $\left\| \mathbb{E}\left[\mathbf{u}_\xi^\star\right] - \mathbf{u}_{\xi=0}^{\mathrm{opt}} \right\|_2 \leq C_\xi \|\widetilde{\boldsymbol{\eta}}_{\xi=0}^{\mathrm{opt}}\|_2$

MSE: $\mathbb{E}\left[\|\mathbf{u}_\xi^\star - \mathbf{u}_{\xi=0}^{\mathrm{opt}}\|_2^2\right] \leq C_\xi^2 \|\widetilde{\boldsymbol{\eta}}_{\xi=0}^{\mathrm{opt}}\|_2^2 + D_\xi \sigma^2,$

$$C_\xi = \frac{\xi M}{s_{\min}(\mathbb{A}(\xi))},\ D_\xi = \mathrm{tr}\left(\mathbb{A}(\xi)^{-1}\Sigma\mathbb{A}(\xi)^{-T}\right),\ \Sigma = \begin{bmatrix} \mathbb{I} & 0 \\ 0 & 0 \end{bmatrix}$$

$C_\xi \uparrow \xi$, and $D_\xi \downarrow \xi$.

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$C_\xi \uparrow \xi$, and $D_\xi \downarrow \xi$.

$\Rightarrow \xi^{\text{opt}}$ is a monotonic increasing function of

$$\frac{\sigma}{\|\widetilde{\boldsymbol{\eta}}_{\xi=0}^{\text{opt}}\|_2} = \frac{\text{meas. inacc.}}{\text{model inacc.}}$$

Adaptivity in ξ key to guarantee accurate estimates.

The optimal ξ minimizes the upper bound for the MSE.

Holdout validation (Kohavi *et al.*, 1995)

Introduce a set of I out-of-sample measurements

$$(\bar{\ell}_1^o, \bar{y}_1), \ldots, (\bar{\ell}_I^o, \bar{y}_I) \Rightarrow (\mathcal{L}_I, \bar{\mathbf{y}})$$

and $\Xi_{\text{train}} = \{\xi_1, \ldots, \xi_Q\} \subset \mathbb{R}_+$.

Solve $\mathbb{A}(\xi_q)\, \mathbf{u}^\star_{\xi_q} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}$, $q = 1, \ldots, Q$.

Return the estimate $u^\star_{\xi^\star}$ such that

$$\xi^\star = \arg\min_{\xi \in \Xi_{\text{train}}} \widehat{MSE}(I) := \frac{1}{I} \|\mathcal{L}_I(u^\star_{\xi_q}) - \bar{\mathbf{y}}\|_2^2.$$

Holdout validation (Kohavi *et al.*, 1995)

Introduce a set of I out-of-sample measurements

$$(\bar{\ell}_1^o, \bar{y}_1), \ldots, (\bar{\ell}_I^o, \bar{y}_I) \Rightarrow (\mathcal{L}_I, \bar{\mathbf{y}})$$

and $\Xi_{\rm train} = \{\xi_1, \ldots, \xi_Q\} \subset \mathbb{R}_+$.

Solve $\mathbb{A}(\xi_q)\,\mathbf{u}_{\xi_q}^\star = \left[\begin{array}{c} \mathbf{y} \\ \mathbf{0} \end{array}\right]$, $q = 1, \ldots, Q$.

Return the estimate $u_{\xi^\star}^\star$ such that

$$\xi^\star = \arg\min_{\xi \in \Xi_{\rm train}} \widehat{MSE}(I) := \frac{1}{I} \|\mathcal{L}_I(u_{\xi_q}^\star) - \bar{\mathbf{y}}\|_2^2.$$

If $\bar{\ell}_i^o = \ell(\cdot, x_i^o, r_{\rm w})$ with $x_i^o \overset{\rm iid}{\sim} {\rm Uniform}(\Omega)$, then $\xi^\star$ approximately minimizes the L^2 error.

Taddei, 2017; Taddei, Penn, Patera, 2017.

Numerical results

- A synthetic example in Acoustics
- A synthetic example in Fluid Mechanics

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Let $u_g(\mu)$ be the solution to

$$\begin{cases} -(1+\epsilon\mu \mathrm{i})\,\Delta u_g(\mu) - \mu^2\, u_g(\mu) = \mu(x_1^2 + e^{x_2}) + \mu g \ \ \text{in}\,\Omega \\ \partial_n u_g(\mu) = 0 \ \ \text{on}\,\partial\,\Omega \end{cases}$$

where $\Omega = (0,1)^2$, $\epsilon = 10^{-2}$.

Bk model: $u^{\mathrm{bk}}(\mu) = u_{g_0}(\mu)$, $\mu \in \mathcal{P}^{\mathrm{bk}} = [2, 10]$, $g_0 \equiv 0$.

True state: $u^{\mathrm{true}} = u_{\bar{g}}(\mu^{\mathrm{true}})$,
$\mu^{\mathrm{true}} \in \mathcal{P}^{\mathrm{bk}}$, $\bar{g}(x) = 0.5(e^{x_1} + \cos(1.3\pi x_2))$.

An acoustic model problem

Let $u_g(\mu)$ be the solution to

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$\mu^{\mathrm{true}} \in \mathcal{P}^{\mathrm{bk}}$, $\bar{g}(x) = 0.5(e^{x_1} + \cos(1.3\pi x_2))$.

Observations: $\{y_m = \mathrm{Gauss}(u^{\mathrm{true}}; x_m^o, r_{\mathrm{w}}) + \epsilon_m\}_{m=1}^M$.

$$\mathrm{Gauss}(v; \bar{x}, r_{\mathrm{w}}) = C(x_m^o) \int_\Omega e^{-\frac{1}{2r_{\mathrm{w}}^2}\|x-\bar{x}\|_2^2}\, v(x)\, dx$$

Details (I): PBDW implementation

Centers: $\{x_m^{\mathrm{o}}\}_m$ deterministic (`SGreedy+approx`),

Choice of ξ: holdout validation
$\{x_i^{\mathrm{o}}\}_i$ drawn randomly (uniform), $I = M/2$;

Background: $\{\mathcal{Z}_N\}_N$ generated using the weak-Greedy algorithm;

Update space: $\{\psi_m(\cdot) = \phi_i(\| \cdot - x_m^o\|_2)\}_m$, $i = 1, 2$
$\phi_1(r) = (1 - r)_+^4(4r + 1)$, csRBF
$\phi_2(r) = \frac{1}{(1+r^2)^2}$ (inverse-multiquadrics)

G Rozza, DBP Huynh, AT Patera, 2008;

H Wendland, 2004.

Details (II): measurement noise

Observations: $y_m = \ell_m^o(u^{\mathrm{true}}) + \epsilon_m$, $\epsilon_m = \epsilon_m^{\mathrm{re}} + \mathrm{i}\epsilon_m^{\mathrm{im}}$,

$$\epsilon_m^{\mathrm{re}} \overset{\mathrm{iid}}{\sim} \mathcal{N}(0, \sigma_{\mathrm{re}}^2), \quad \epsilon_m^{\mathrm{im}} \overset{\mathrm{iid}}{\sim} \mathcal{N}(0, \sigma_{\mathrm{im}}^2);$$

$$\sigma_{\mathrm{re}} = \frac{1}{\mathrm{SNR}} \times \mathrm{std}\left(\left\{\Re\left(\ell_m^o(u^{\mathrm{true}})\right)\right\}_{m=1}^M\right);$$

$$\sigma_{\mathrm{im}} = \frac{1}{\mathrm{SNR}} \times \mathrm{std}\left(\left\{\Im\left(\ell_m^o(u^{\mathrm{true}})\right)\right\}_{m=1}^M\right).$$

Details (II): measure of performance

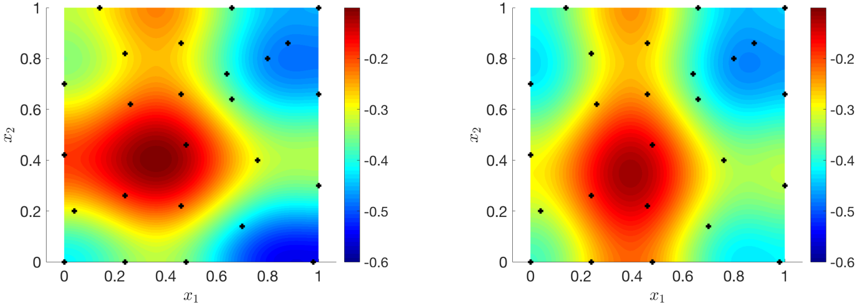
$$E_{\text{avg}}^{\text{rel}} = \frac{1}{|\mathcal{P}_{\text{train}}^{\text{bk}}|} \sum_{\mu \in \mathcal{P}_{\text{train}}^{\text{bk}}} \frac{\| u^{\text{true}}(\mu) - u_\xi^\star(\mu) \|_{L^2(\Omega)}}{\| u^{\text{true}}(\mu) \|_{L^2(\Omega)}},$$

$\mathcal{P}_{\text{train}}^{\text{bk}} \subset [2, 10]$, $|\mathcal{P}_{\text{train}}^{\text{bk}}| = 10$.

If $\text{SNR} < \infty$ (noisy measurements), computations of $\| u^{\text{true}}(\mu) - u_\xi^\star(\mu) \|_{L^2(\Omega)}$ are averaged over $K = 35$ trials.

Visualization ($N = 6, M = 25, \mu^{\text{true}} = 8.28, r_{\text{w}} = 0.01$)

1. Background approximation: compute $z_\xi^\star$.



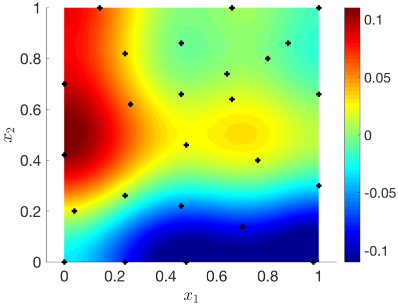
(a) $\Re\left(u^{\text{true}}\right)$ (b) $\Re\left(z_\xi^\star\right)$

Update space is built using inverse multiquadrics.

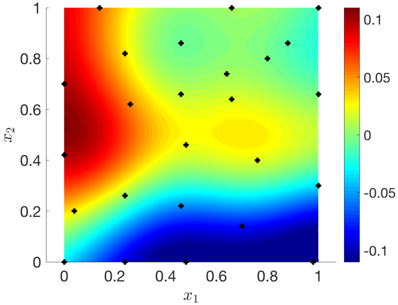
$z_\xi^\star$ can be computed directly by assembling the Schur's complement associated with $\mathbb{A}(\xi)$: this leads to a two-step procedure for the computation of the PBDW estimate.

Visualization ($N = 6$, $M = 25$, $\mu^{\mathrm{true}} = 8.28$, $r_{\mathrm{w}} = 0.01$)

2. Correction: compute $\eta_\xi^\star$.



(a) $\mathfrak{R}\left(u^{\mathrm{true}} - z_\xi^\star\right)$

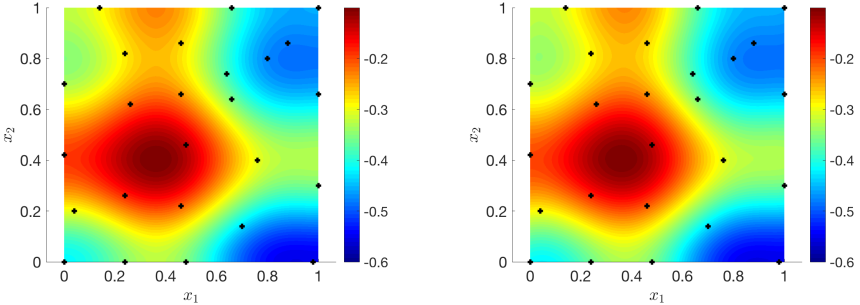


(b) $\mathfrak{R}\left(\eta_\xi^\star\right)$

Update space is built using inverse multiquadrics.

$z_\xi^\star$ can be computed directly by assembling the Schur's complement associated with $\mathbb{A}(\xi)$: this leads to a two-step procedure for the computation of the PBDW estimate.

3. Final estimate: compute $u_\xi^\star = z_\xi^\star + \eta_\xi^\star$.



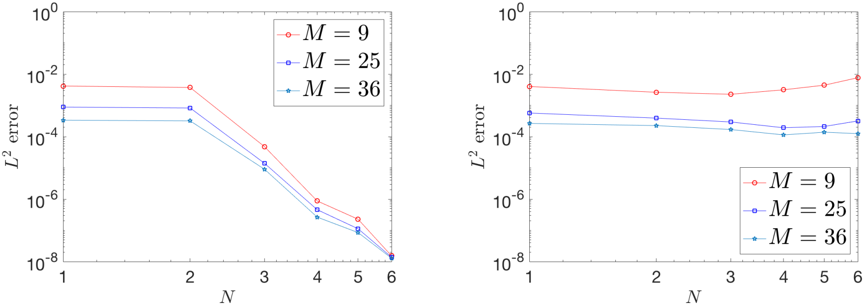
(a) $\Re\left(u^{\mathrm{true}}\right)$ (b) $\Re\left(u_\xi^\star\right)$

Update space is built using inverse multiquadrics.

$z_\xi^\star$ can be computed directly by assembling the Schur's complement associated with $\mathbb{A}(\xi)$: this leads to a two-step procedure for the computation of the PBDW estimate.

N convergence ($\mathrm{SNR} = \infty$, $r_{\mathrm{w}} = 0.05$)

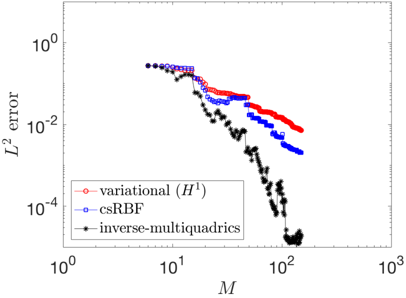
If $u^{\mathrm{true}} \in \mathcal{M}^{\mathrm{bk}}$, we observe exponential convergence in N; if $u^{\mathrm{true}} \notin \mathcal{M}^{\mathrm{bk}}$, increasing N does not asymptotically improve accuracy.



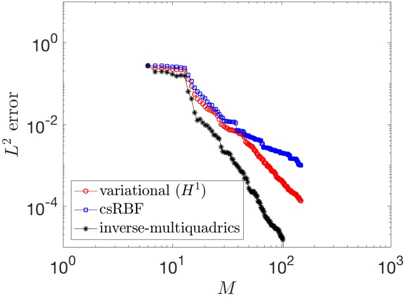
(a) $u^{\mathrm{true}} \in \mathcal{M}^{\mathrm{bk}}$ (b) $u^{\mathrm{true}} \notin \mathcal{M}^{\mathrm{bk}}$

M convergence: $(\mathrm{SNR} = \infty,\ N = 6)$

Use of inverse-multiquadrics significantly improves performance, particularly for small values of r_{w}.



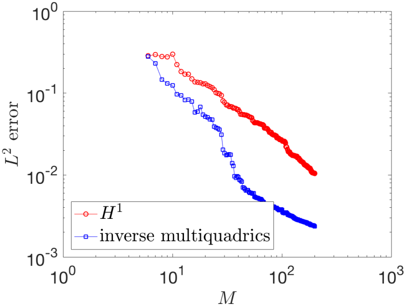
(a) $r_{\mathrm{w}} = 0.01$



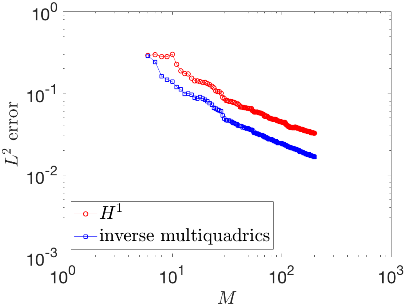
(b) $r_{\mathrm{w}} = 0.05$

M convergence: $(\mathrm{SNR} < \infty,\ N = 4,\ r_{\mathrm{w}} = 0.01)$

Use of inverse-multiquadrics significantly improves performance also for noisy measurements.

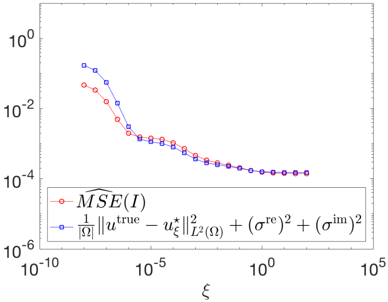


(a) $\mathrm{SNR} = 100$

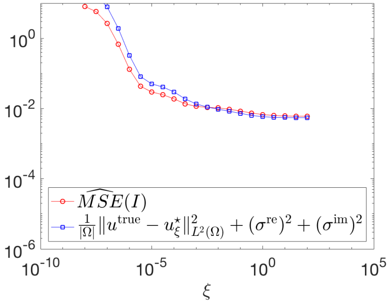


(b) $\mathrm{SNR} = 10$

Details: $M = 100$, $I = 50$, $N = 5$, $r_{\mathrm{w}} = 0.01$, update based on inverse multiquadrics.



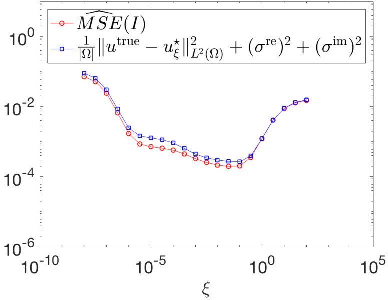
(a) $\mathrm{SNR} = 20$



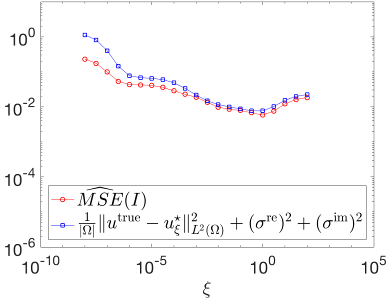
(b) $\mathrm{SNR} = 3.33$

Interpretation of the hyper-parameter ξ: $u^{\text{true}} \notin \mathcal{M}^{\text{bk}}$

Details: $M = 100$, $I = 50$, $N = 5$, $r_{\mathrm{w}} = 0.01$, update based on inverse multiquadrics.



(a) SNR $= 20$



(b) SNR $= 3.33$

Numerical results

- A synthetic example in Acoustics
- A synthetic example in Fluid Mechanics

A Fluid Mechanics problem

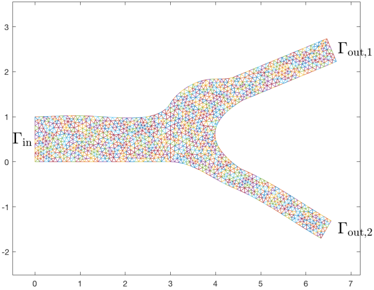
Let $(u,p) = (u_g(\mathrm{Re}), p_g(\mathrm{Re}))$ be the solution to

$$(u\cdot\nabla)u - \nabla\cdot\sigma_{\mathrm{Re}}(u,p) = 0$$

$$\nabla\cdot u = 0$$

$$\sigma_{\mathrm{Re}}(u,p)n = 0 \quad \text{on } \Gamma_{\mathrm{out}}$$

$$u|_{\Gamma_{\mathrm{in}}} = g\, e_1, \qquad u|_{\Gamma_{\mathrm{hom}}} = 0$$



Bk model: $g(x_2) = 4(1-x_2)x_2,\ \mathrm{Re}\in[50,350]$.

True state: $g(x_2) = 4(1-x_2)x_2(1+0.1\sin(2\pi x_2))$,

Observations: $y_m = \underbrace{C(x_m^o)\int_\Omega e^{-\frac{1}{2r_{\mathrm{w}}^2}\|x-x_m^o\|_2^2}\, u^{\mathrm{true}}(x)\,dx}_{=:\ell_m^o(u^{\mathrm{true}})=\mathrm{Gauss}(u^{\mathrm{true}};x_m^o,r_{\mathrm{w}})}$.

Details (I): PBDW implementation

Centers: $\{x_m^{\mathrm{o}}\}_m$ deterministic (`SGreedy+approx`),

Choice of ξ: $\xi \to 0^+$

Background: $\{\mathcal{Z}_N\}_N$ generated using POD

Update space:

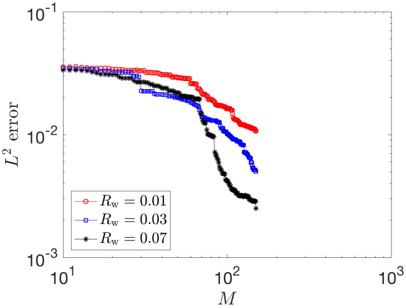
$$\{\psi_{2m-i}(\cdot) = R_{\mathcal{X}}\mathrm{Gauss}(\cdot \bullet e_i, x_m^o, R_{\mathrm{w}})\}_{m=1,\ldots,M, i=1,2},$$

$$\mathcal{X} = \{v \in [H^1(\Omega)]^2 : \nabla \cdot v = 0, \, v|_{\Gamma_{\mathrm{hom}}} = 0\}$$

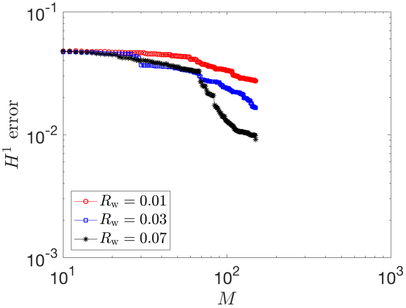
$$\| \cdot \|_{\mathcal{X}} = \| \nabla \cdot \|_{L^2(\Omega)}.$$

$\psi_1, \ldots, \psi_{2M}$ are divergence-free and satisfy homogeneous conditions on $\Gamma_{\mathrm{hom}} = \partial\Omega \setminus (\Gamma_{\mathrm{in}} \cup \Gamma_{\mathrm{out}})$.

Increasing R_{w} leads to an improvement in accuracy.



(a) L^2



(b) H^1

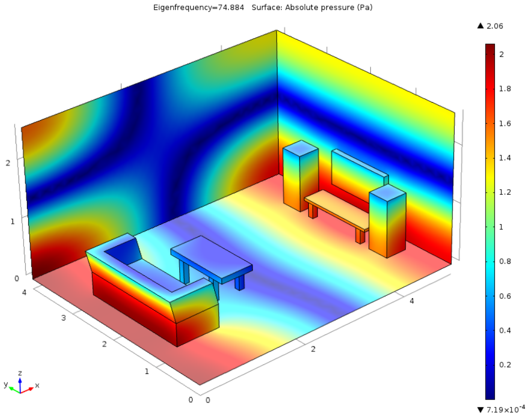
Localized state estimation: $\Omega \subset \Omega^{\mathrm{bk}}$

- Methodology
- Numerical results

Localized state estimation: $\Omega \subset \Omega^{\mathrm{bk}}$

- Methodology
- Numerical results

Objective: estimate the state in a subregion Ω of the original domain Ω^{pb}.



[1]Photo credits: www.comsol.com

Localization strategy (Taddei & Patera, SISC, accepted)

Strategy: restrict computations to $\Omega^{\rm bk}$, $\Omega \subset \Omega^{\rm bk} \subset \Omega^{\rm pb}$.

uncertainty in global inputs $\Rightarrow$ uncertainty at port $\Gamma^{\rm in}$.

Solution manifold

$$\mathcal{M}^{\rm bk} = \{ u_g^{\rm bk}(\mu)|_{\Omega} : \quad \underbrace{\mu \in \mathcal{P}^{\rm bk}}_{\text{parameters}} \quad \underbrace{g \in \mathcal{T} = \mathcal{T}(\Gamma^{\rm in})}_{\text{boundary conditions}} \quad \}$$

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Strategy: restrict computations to Ω^{bk}, $\Omega \subset \Omega^{\mathrm{bk}} \subset \Omega^{\mathrm{pb}}$.

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Solution manifold

$$\mathcal{M}^{\mathrm{bk}} = \{ u_g^{\mathrm{bk}}(\mu)|_{\Omega} : \underbrace{\mu \in \mathcal{P}^{\mathrm{bk}}}_{\text{parameters}} \quad \underbrace{g \in \mathcal{T} = \mathcal{T}(\Gamma^{\mathrm{in}})}_{\text{boundary conditions}} \}$$

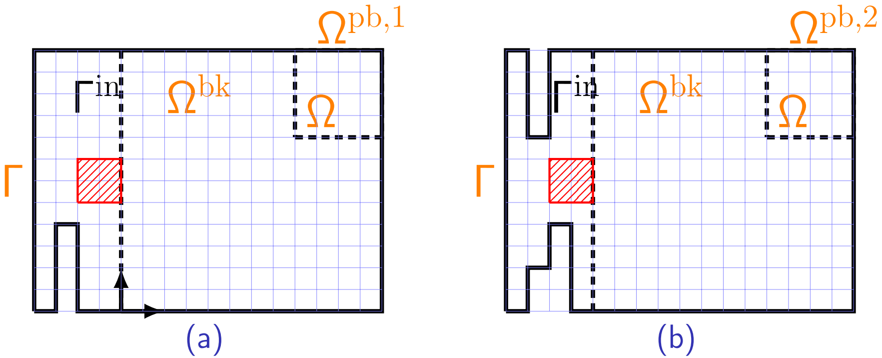
Refined objective: determine rapidly convergent spaces $\mathcal{Z}_N$ to approximate $\mathcal{M}^{\mathrm{bk}}$

Fundamental question: is the manifold reducible?

($\leftrightarrow$ evanescence);

Challenge: $\mathcal{P}^{\mathrm{bk}} \times \mathcal{T}$ is infinite-dimensional.

A model problem in Acoustics



The red region is associated with a volumetric acoustic source.

A model problem in Acoustics

We consider the bk mathematical model:

$$\begin{cases} -(1+\epsilon \mathrm{i})\Delta u_g(\mu) - \mu^2 u_g(\mu) = 0 & \text{in } \Omega^{\mathrm{bk}}; \\ \partial_n u_g(\mu) = 0 & \text{on } \partial\Omega^{\mathrm{bk}} \setminus \Gamma^{\mathrm{in}}; \\ u_g(\mu) = g & \text{on } \Gamma^{\mathrm{in}}; \end{cases}$$

while the true field satisfies ($j = 1, 2$)

$$\begin{cases} -(1+\epsilon \mathtt{i})\Delta u_j^{\mathrm{true}}(\mu) - \mu^2 u_j^{\mathrm{true}}(\mu) = f & \text{in } \Omega^{\mathrm{pb},j}; \\ \partial_n u_j^{\mathrm{true}}(\mu) = 0 & \text{on } \partial\Omega^{\mathrm{pb},j} \setminus \Gamma; \\ u_j^{\mathrm{true}}(\mu) = h^{\mathrm{true}} & \text{on } \Gamma; \end{cases}$$

Note that $u_1^{\mathrm{true}}, u_2^{\mathrm{true}} \in \mathcal{M}^{\mathrm{bk}}$.

$\mathcal{P}^{\mathrm{bk}} = \{\bar{\mu}\}$: transfer eigenproblem (Pinkus, 1985)

Define $\mathcal{T} = H^{1/2}(\Gamma^{\mathrm{in}})$, $\mathcal{Y} = H^1(\Omega)$, and

$$A : \mathcal{T} \to \mathcal{Y} \text{ s.t. } u_g(\bar{\mu})|_\Omega = A(g)$$

Transfer eigenpb: $(A(\phi_n), A(g))_{\mathcal{Y}} = \lambda_n (\phi_n, g)_{\mathcal{T}} \quad \forall\, g$

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Transfer eigenpb: $(A(\phi_n), A(g))_{\mathcal{Y}} = \lambda_n (\phi_n, g)_{\mathcal{T}} \quad \forall\, g$

Proposition: if A is *compact*, $\mathcal{Z}_N^{\mathrm{te}} = \mathrm{span}\{A(\phi_n)\}_n$ (*transfer eigenspace*) minimizes the N-width:

$$d_N(A) := \inf_{Z_N \subset \mathcal{Y},\, \dim(Z_N)=N} \sup_{g \in \mathcal{T}} \frac{\| A(g) - \Pi_{Z_N}^{\mathcal{Y}} A(g) \|_{\mathcal{Y}}}{\| g \|_{\mathcal{T}}}$$

furthermore, $d_N(A) = \sqrt{\lambda_{N+1}}$.

The map A is compact for a broad class of linear elliptic PDEs (Helmholtz, elastodynamics, Stokes (velocity),...)

Practical computation of the Transfer Eigenspace

Introduce $\mathcal{T}_{\mathcal{N}_{\text{in}}} = \operatorname{span}\{g_i\}_{i=1}^{\mathcal{N}_{\text{in}}}$. Estimate $\{(\phi_n, \lambda_n)\}_n$ as

$$\bar{\phi}_n = \sum_{i=1}^{\mathcal{N}_{\text{in}}} \left(\bar{\boldsymbol{\phi}}_n\right)_i g_i, \text{ where } \mathbb{U}\bar{\boldsymbol{\phi}}_n = \bar{\lambda}_n \mathbb{T}\bar{\boldsymbol{\phi}}_n;$$

$\mathbb{U}_{i,i'} = (A(g_i), A(g_{i'}))_{\mathcal{Y}}$, $\mathbb{T}_{i,i'} = (g_i, g_{i'})_{\mathcal{T}}$

[2]Randomization techniques can be used to reduce offline costs; see Buhr & Smetana, *Randomized Local Model Order Reduction*, SISC, accepted.

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$\mathbb{U}_{i,i'} = (A(g_i), A(g_{i'}))_{\mathcal{Y}}$, $\mathbb{T}_{i,i'} = (g_i, g_{i'})_{\mathcal{T}}$

If $\mathbb{T} = \mathbb{1}$ (i.e., $\{g_i\}_i$ orthonormal in $\mathcal{T}$) $\Rightarrow$ TE = POD

$$\frac{\|A(g) - \Pi^{\mathcal{Y}}_{\mathcal{Z}^{\text{te}}_N} A(g)\|_{\mathcal{Y}}}{\|g\|_{\mathcal{T}}} \leq \|A\|_{\mathcal{L}(\mathcal{T}^{\perp}_{\mathcal{N}_{\text{in}}},\mathcal{Y})} \frac{\|\Pi^{\mathcal{T}}_{\mathcal{T}^{\perp}_{\mathcal{N}_{\text{in}}}} g\|_{\mathcal{T}}}{\|g\|_{\mathcal{T}}} + \sqrt{\bar{\lambda}_{N+1}}$$

$\mathcal{T}_{\mathcal{N}_{\text{in}}}$ should be chosen to reduce $\|A\|_{\mathcal{L}(\mathcal{T}^{\perp}_{\mathcal{N}_{\text{in}}},\mathcal{Y})}$.

Here, we choose polynomials[2].

[2] Randomization techniques can be used to reduce offline costs; see Buhr & Smetana, *Randomized Local Model Order Reduction*, SISC, accepted.

$\mathcal{P}^{\mathrm{bk}} \neq \{\bar{\mu}\}$: transfer eigenproblem + POD

Given $\mu^1, \ldots, \mu^{n_{\mathrm{train}}} \in \mathcal{P}^{\mathrm{bk}}$,

compute $\mathcal{Z}_N^{\mathrm{te}}(\mu^i) = \mathrm{span}\{A(\phi_n^i; \mu^i)\}_{n=1}^N$

Apply POD to $\{A(\phi_n^i; \mu^i)\}_{i=1,\ldots,n_{\mathrm{train}}, n=1,\ldots,N}$

$\mathcal{P}^{\rm bk} \neq \{\bar{\mu}\}$: transfer eigenproblem + POD

Given $\mu^1, \ldots, \mu^{n_{\rm train}} \in \mathcal{P}^{\rm bk}$,

compute $\mathcal{Z}_N^{\rm te}(\mu^i) = {\rm span}\{A(\phi_n^i; \mu^i)\}_{n=1}^N$

Apply POD to $\{A(\phi_n^i; \mu^i)\}_{i=1,\ldots,n_{\rm train}, n=1,\ldots,N}$

The approach can be seen as a Hierarchical Approximate POD.

$\{\phi_n^i\}_{i=1,\ldots,n_{\rm train}, n=1,\ldots,N}$ should satisfy $\|\phi_n^i\|_{\mathcal{T}} = 1$.

The approach is affordable only for moderate values of $n_{\rm train}$ ($\Rightarrow$ low-dimensional parameterizations).

Himpe, Leibner, Rave, *Hierarchical Approximate Proper Orthogonal Decomposition*, Arxiv, 2016.

Localized state estimation: $\Omega \subset \Omega^{\mathrm{bk}}$

- Methodology
- Numerical results

Observations: $y_m = \mathrm{Gauss}(u^{\mathrm{true}}; x_m^o, r_{\mathrm{w}})$

Update space: $\{\psi_m(\cdot) = \phi(2\| \cdot - x_m^o\|_2)\}_{m=1}^M$

$$\phi(r) = \frac{1}{(1+r^2)^2} \text{ (inverse multiquadrics)}$$

Port space: $\mathcal{T}_{\mathcal{N}_{\mathrm{in}}} = \mathrm{span}\{\mathcal{L}_n\}_{n=1}^{\mathcal{N}_{\mathrm{in}}}$, $\mathcal{N}_{\mathrm{in}} = 20$

$\mathcal{L}_n$ n-th Legendre polynomial on Γ^{in}

Observations: $y_m = \mathrm{Gauss}(u^{\mathrm{true}}; x^o_m, r_{\mathrm{w}})$

Update space: $\{\psi_m(\cdot) = \phi(2\| \cdot - x^o_m\|_2)\}_{m=1}^{M}$

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Port space: $\mathcal{T}_{\mathcal{N}_{\mathrm{in}}} = \mathrm{span}\{\mathcal{L}_n\}_{n=1}^{\mathcal{N}_{\mathrm{in}}}$, $\mathcal{N}_{\mathrm{in}} = 20$

$\mathcal{L}_n$ n-th Legendre polynomial on Γ^{in}

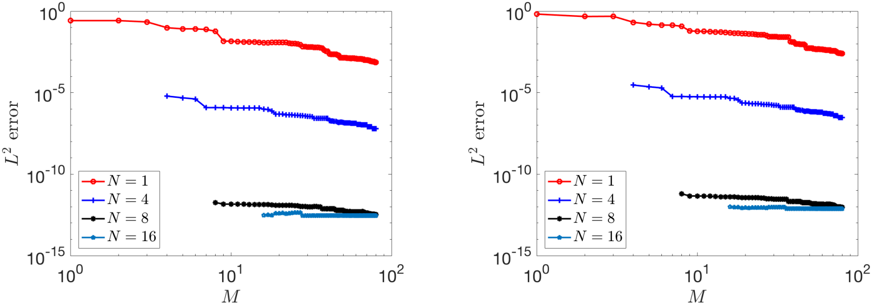
We choose observation centers using `SGreedy+approx`.

We measure performance by computing the averaged relative L^2 error.

$h^{\mathrm{true}}(x_2) = \sin(k\pi x_2)$, $k = 1, 2, 3$.

M convergence: $\mathcal{P}^{\text{bk}} = \{\bar{\mu} = 2\}$ ($\text{SNR} = \infty$, $r_{\text{w}} = 0.02$)

For $\bar{\mu} = 2$, solution to the transfer eigenproblem generates fast-converging approximation spaces for the problem at hand.

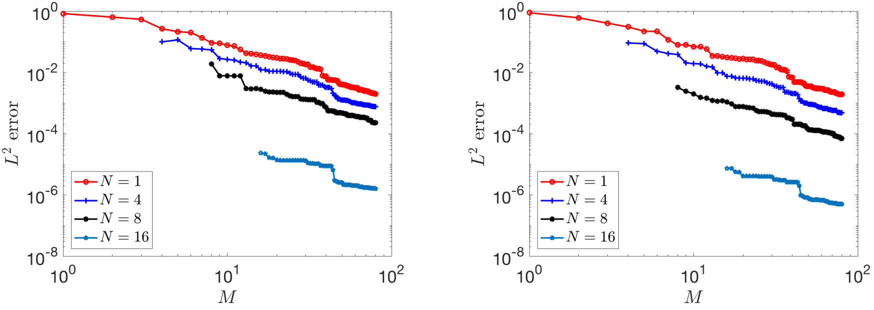


(a) $\Omega^{\text{pb},1}$ (b) $\Omega^{\text{pb},2}$

Test: we consider

equispaced $\mu^1, \ldots, \mu^{n_{\rm train}}$ in $\mathcal{P}^{\rm bk}$ for training, $n_{\rm train} = 11$

randomly-chosen $\mu^1, \ldots, \mu^{n_{\rm test}} \in \mathcal{P}^{\rm bk}$ for testing, $n_{\rm test} = 5$.



(a) $\Omega^{\rm pb,1}$ (b) $\Omega^{\rm pb,2}$

Summary and perspectives

Summary

PBDW is a MOR approach for the efficient integration of

- parametrized mathematical models, and
- experimental observations

for state estimation.

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PBDW is a MOR approach for the efficient integration of

- parametrized mathematical models, and
- experimental observations

for state estimation.

MOR allows the efficient treatment of parametrized mathematical models.

User-defined updates provide the PBDW formulation with additional flexibility.

A priori analysis clarifies the role of several elements of the formulation.

PBDW is restricted to deterministic backgrounds, stationary processes, and fixed domains.

Possible extensions include

probabilistic backgrounds,

$$\mu \sim \mathbb{P}_\mu(\mathcal{P}^{\rm bk}) \Rightarrow \boldsymbol{\alpha} \sim \mathbb{P}_\alpha(\mathbb{R}^N)$$

time-dependent problems,

space-time recovery based on sparse measurements,

estimation in movable domains,

e.g., internal flows subjected to geometric uncertainty.

Thank you for your attention!

Backup slides

Scattered data approximation with RBFs[3]

1. Choose the PD RBF $\Phi : \mathbb{R}_+ \to \mathbb{R}_+$
2. Characterize the properties of $\mathcal{X} = \mathcal{N}_\Phi$ for analysis.

Similarity: infinite-dimensional formulation used only for analysis.

Key difference: $\mathcal{X} = \mathcal{N}_\Phi$ and its inner product do **not** depend on $x_1^o, \ldots, x_M^o$.

[3] PBDW and RBF scattered data approximation are equivalent for $\mathcal{Z}_N = \emptyset, \{\ell_m^o = \delta_{x_m^o}\}_{m=1}^M$.