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

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

$\ell_1^o, \dots, \ell_M^o$ linear functionals,
$\mathcal{L}_M = [\ell_1^o, \dots, \ell_M^o]$

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^{true} as

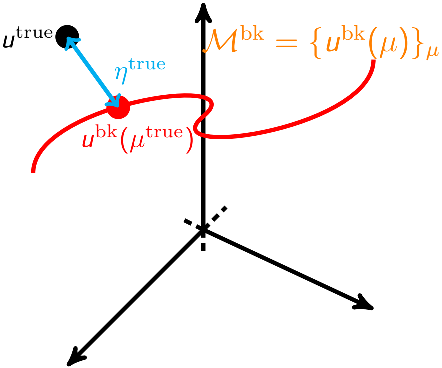
$$u^{\mathrm{true}} = u^{\mathrm{bk}}(\mu^{\mathrm{true}}) + \eta^{\mathrm{true}},\ \mu^{\mathrm{true}} \in \mathcal{P}^{\mathrm{bk}},\ \eta^{\mathrm{true}} \in \mathcal{U}.$$

$$\mu^{\mathrm{true}} := \arg\min_{\mu} \| u^{\mathrm{true}} - u^{\mathrm{bk}}(\mu) \|$$

addresses uncertainty in μ

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

addresses model uncertainty



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

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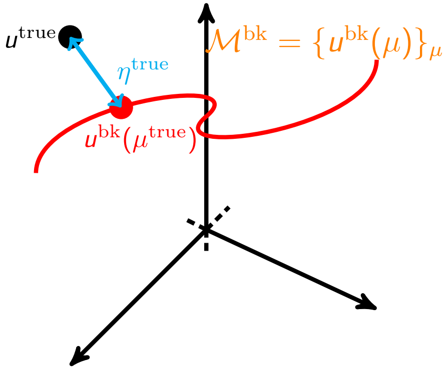

PSM: $$\min_{(\mu,\eta)\in\mathcal{P}^{\mathrm{bk}}\times\mathcal{U}} \underbrace{\xi\|\eta\|^2}_{\text{penalty}} + \underbrace{V_M\left(\mathcal{L}_M(u^{\mathrm{bk}}(\mu)+\eta) - \mathbf{y}\right)}_{\text{data misfit}}$$

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

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

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

Relaxation: PSM $\rightarrow$ PBDW

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

Then, obtain the **PBDW statement**:

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

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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 $u^{\rm bk}$:

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

where $N \leq M$ 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^{bk}:

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

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

Data compression: given the *bk manifold*

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

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

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

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

General formulation:

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

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

Maday, Patera, Penn, Yano, *A parameterized-background data-weak approach to variational data assimilation: formulation, analysis, and application to acoustics*, IJNME, 2015

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Taddei, Patera, *A localization strategy for Data Assimilation; application to state estimation and parameter estimation*, SISC, (accepted).

Maday, Taddei, *Adaptive PBDW approach to state estimation: noisy observations; user-defined update spaces.*, (submitted).

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

Hammond, Chakir, Bourquin, Maday, *PBDW: a non-intrusive reduced basis data assimilation method and its application to outdoor air quality models*, (submitted).

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

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

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

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

Maday, Taddei, *Adaptive PBDW approach to state estimation: noisy observations; user-defined update spaces*, (submitted).

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

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

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

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

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

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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.

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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 $\psi_1, \dots, \psi_M$ for local measurements

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

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

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

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

   simple treatment of strong BCs

Equivalence between variational and user-defined updates

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

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

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

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

Error analysis for perfect measurements

Introduce

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

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

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

Then,

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

where $C(\xi) \to 0$ as $\xi \to 0^+$.

Numerical results

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

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An acoustic model problem

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

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

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

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

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

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

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

Details (II): measure of performance

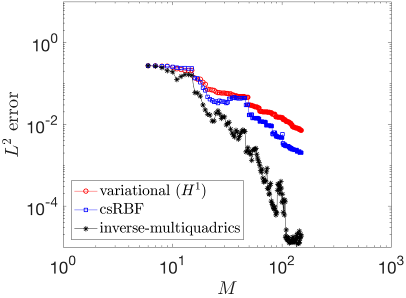
$$E_{\text{avg}}^{\text{rel}} = \frac{1}{|\mathcal{P}_{\text{train}}^{\text{bk}}|} \sum_{\mu \in \mathcal{P}_{\text{train}}^{\text{bk}}} \frac{\| u^{\text{true}}(\mu) - u_{\xi}^{\star}(\mu) \|_{L^2(\Omega)}}{\| u^{\text{true}}(\mu) \|_{L^2(\Omega)}},$$

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

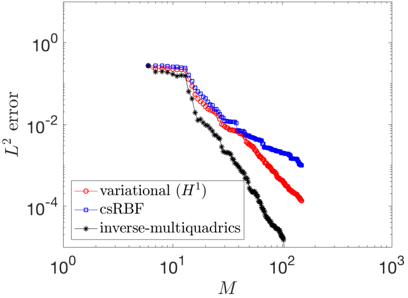
If $\text{SNR} < \infty$ (noisy measurements), computations of $\| u^{\text{true}}(\mu) - u_{\xi}^{\star}(\mu) \|_{L^2(\Omega)}$ are averaged over $K = 35$ trials.

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

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



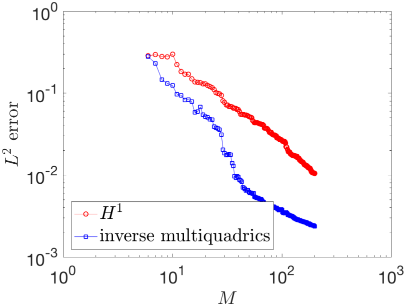
(a) $r_{\mathrm{w}} = 0.01$



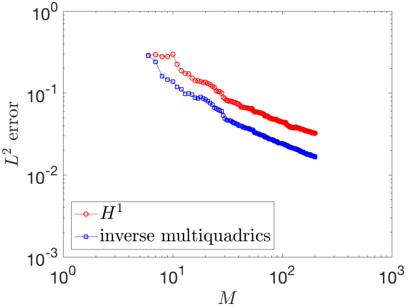
(b) $r_{\mathrm{w}} = 0.05$

$M-$ 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) $\mathrm{SNR} = 10$

Numerical results

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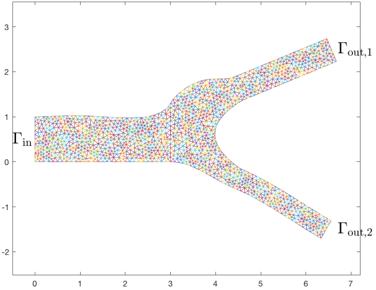
- A synthetic example in Fluid Mechanics

A Fluid Mechanics problem

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

$$\begin{cases} (u \cdot \nabla)u - \nabla \cdot \sigma_{\mathrm{Re}}(u, p) = \\ \nabla \cdot u = 0 \\ \sigma_{\mathrm{Re}}(u, p)n = 0 \quad \text{on } \Gamma_{\mathrm{out}} \\ u|_{\Gamma_{\mathrm{in}}} = g\, e_1, \quad u|_{\Gamma_{\mathrm{hom}}} = 0 \end{cases}$$



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

Choice of ξ: $\xi \to 0^+$

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

Update space:

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

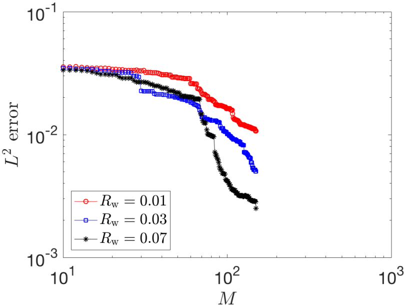
$$\mathcal{X} = \{v \in [H^1(\Omega)]^2 : \nabla \cdot v = 0, \; v|_{\Gamma_{\rm hom}} = 0\}$$

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

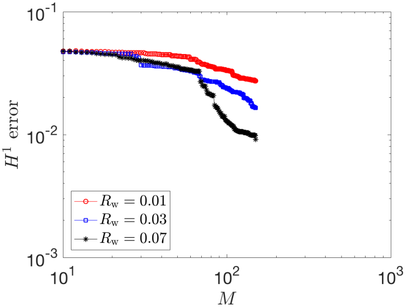
$\psi_1, \ldots, \psi_{2M}$ are divergence-free and satisfy homogeneous conditions on $\Gamma_{\rm hom} = \partial\Omega \setminus (\Gamma_{\rm in} \cup \Gamma_{\rm out})$.

$M-$ convergence: $(\mathrm{SNR} = \infty,\ N = 5,\ r_{\mathrm{w}} = 0.01)$

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



(a) L^2



(b) H^1

Conclusions

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for state estimation.

MOR allows the efficient treatment of parametrized mathematical models.

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

Thank you for your attention!

Backup slides

Connection with Kernel methods

Scattered data approximation with RBFs[1]

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 $x_1^o, \ldots, x_M^o$.

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