Reduced-Basis method for 4DVar data assimilation

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Outline

Problem setting: 4Dvar parametrized

Reduced-Basis: error estimate + greedy projection

Numerical tests: error effectivity and decay rate

A Gaussian linear parametric SPDE model

Advection-diffusion of a quantity c with Gaussian source

$$(\partial_t + u \cdot \nabla - \nu \Delta) c = f + \dot{B}$$

is parametrized by 2 kinds of input:

- boundary conditions like $c(t=0)$, $\dot{B} := \left(\dot{B}(t)\right)_{t \in (0,T)}$
- process *parameters* like ν

Having in mind a *two-step* Data Assimilation (DA) procedure

1. given ν, fit $c(t=0)$, $\dot{B}$ to "data about $c(t;\nu)$, $t \in [0,T)$"
2. given $\{c(t;\nu), t \in [0,T); \nu \in \Lambda\}$ "optimize" ν

the *Reduced-Basis* method can decrease computational costs: $c(t=0)$, $\dot{B}$ have to be fit *for many values of the parameter* ν.

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DA by **smoothing** in a discrete setting

In practice, one considers calibrating the input of a space-discrete model at discrete times $t^n \in [0, N\Delta t]$

$$(m + \Delta t \; a(\nu))c^n = m \; c^{n-1} + \Delta t \; f^n + \sqrt{\Delta t} \; g_j w_j^n$$

which we rewrite in standard DA notations

$$x_n = M(\nu)x_{n-1} + f_n + \eta_n \qquad \eta_n \sim \mathcal{N}(0, Q_n)$$

One DA approach using $z_n = H \; x_n + \epsilon_n$, $\epsilon_n \sim \mathcal{N}(0, R_n)$ maximizes the *posterior* probability law

$$x_0, \ldots, x_N | z_0 = z_0^d, \ldots, z_N = z_N^d \sim \mathcal{N}(x^s, P^s)$$

using a *background* as prior $mc^{-1} + \Delta t \; f_0$ (=:*smoothing*)

$$x_0 \sim \mathcal{N}(x_0^f := Mx_{-1} + f_0, P_0^f := Q_0)$$

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MAP of $\mathcal{N}(x^s, P^s)$: quadratic minimization

$$p(x_0 \dots x_N | z_0 \dots z_N) \propto \prod_{k=0}^{N} p(z_k|x_k) p(x_k|x_{k-1}) \text{ MAP } \textit{minimizes}$$

$$\begin{aligned} J(x_0 \dots x_N) := \sum_{n=0}^{N} (Hx_n - z_n^d)^T R_n^{-1} (Hx_n - z_n^d) \\ + \sum_{n=1}^{N} (x_n - Mx_{n-1} - f_{n-1})^T Q_n^{-1} (x_n - Mx_{n-1} - f_{n-1}) \\ + (x_0 - x_0^f)^T Q_0^{-1} (x_0 - x_0^f) \end{aligned} \tag{1}$$

the so-called **weak 4DVar** computational problem:
a large (invertible) linear system *parametrized by* ν in $M(\nu)$.

4DVar with parameter: cost decreased by RB

4DVar is computationally expensive, especially if $N \gg 1$.

Computing $x^s(\nu)$ for many ν is *very* expensive.

A *Reduced Basis (RB)* approximation $\tilde{x}^s(\nu) \approx x^s(\nu)$
decreases the computational cost of $x^s(\nu)$
after a *learning stage* has exploited enough variations in ν.

A good *estimator* for $\tilde{x}^s(\nu) - x^s(\nu)$ is crucial to a fast learning stage.

Note : in practice, the 4DVar saddle-point system is often reduced but *without error control*

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Reduced Basis $\approx$ "hyper-Galerkin", $\Rightarrow$ error estimate !

When $x_n = Mx_{n-1} + f_n + \eta_n$ results from PDE discretization

$$(m + \Delta t\ a)c^n = mc^{n-1} + \Delta t\ f^n + \sqrt{\Delta t}\ g_j w_j^n$$

proj. $x \approx \hat{x} = Xy$ onto *Reduced Basis* $\mathrm{rank}(X) \ll N \times \sharp(d.o.f.)$

$$(\hat{m} + \Delta t\ \hat{a})\hat{c}^n = \hat{m}\hat{c}^{n-1} + \Delta t\ \hat{f}^n + \sqrt{\Delta t}\ \hat{g}_j w_j^n$$

is computationally cheaper ... once X has been identified !

Using *residuals*: $(m + \Delta t\ a)e_c^n = me_c^{n-1} + \Delta t\ r_c^n + \Delta t\ e_B^n$,
greedy algorithms construct X incrementally, inspecting a sample of $\|e_c^N(\nu)\|^2 := \|c^N - X\hat{c}^N\|_{a_0}^2$ through *estimates*:

$$(\beta_m + \tfrac{\Delta t}{4}\beta_a)\|e_c^n\|^2 \le \beta_m \|e_c^{n-1}\|^2 + \tfrac{\Delta t}{2}\beta_a^{-1}\|r_c^n\|_{a_0'}^2 + \tfrac{\Delta t}{2} C_m \|e_B^n\|_m^2$$

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$$\beta_a \sum_{n=1}^{N} \|e_c^n\|^2 \leq \beta_m \|e_c^0\|^2 + 2\beta_a^{-1} \sum_{n=1}^{N} \|r_c^n\|_{a_0'}^2 + 2C_m \sum_{n=1}^{N} \|e_B^n\|_m^2 := \Delta$$

Reduced Basis construction for parabolic PDEs

Standard RB uses a *POD-greedy algorithm*:

1. $X = \mathrm{span}\{\zeta_1\}$ using
   ζ_1 *principal component* of $c^1(\nu_1), \ldots, c^N(\nu_1)$ at ν_1
2. While $\max_{\nu \in \Lambda_{train}} \Delta(\nu) > \varepsilon$, $X = X \cup \{\zeta\}$ using
   POD modes ζ of $c^1(\bar{\nu}), \ldots, c^N(\bar{\nu})$ at $\bar{\nu} \in \underset{\nu \in \Lambda}{\mathrm{argmax}} \Delta(\nu)$

Key to the reduction are:

- the "linear" dimension of $\{c^1(\nu), \ldots, c^N(\nu); \nu \in \Lambda\}$
- the convergence rate of the greedy algorithm
- the accuracy in error estimate

Let us *specialize* to 4DVar

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Reduced Basis construction for 4DVar: estimate

Duality: rewrite J with $\sum_{n=1}^{N}(p^n)^T Q_n^{-1} p^n$ and

$$+\left((m+\Delta t\ a)c^n - mc^{n-1} - \Delta t\ f^n - \sqrt{\Delta t}\, g_j w_j^n\right)^T p^n$$

so 4Dvar rewrites as a system for c^n, p^n with $p^N = 0$ and

$$(m+\Delta t\ a)p^{n-1} = mp^n + H^T R_n^{-1}(z_n^d - Hc^n)$$

which can be treated by RB like the (forward) eq. for c^n

$$\sum_{n=1}^{N} \|e_p^N\|^2 \le \beta_a^{-1}\left(2\beta_a^{-1}\sum_{n=1}^{N}\|r_p^n\|_{a_0'}^2 + 2C_m C_{H^T R^{-1} H}\sum_{n=1}^{N}\|e_c^n\|^2\right)$$

Reduced Basis construction for 4DVar: greedy

$$\|e_c^0\|^2 + \sum_{n=1}^{N} \|e_B^n\|^2 \lesssim \beta_a^{-2} \left(\sum_{n=1}^{N} \|r_p^n\|_{a'_0}^2 + \sum_{n=1}^{N} \|r_c^n\|_{a'_0}^2 \right) := \Delta'$$

allows 4DVar RB to use a *new* POD-greedy given $\epsilon > 0$:

1. $X = \mathrm{Span}\{\zeta_1, \zeta_2\}$
   ζ_1 *principal component* of $c^1(\nu_1), \dots, c^N(\nu_1)$
   ζ_2 *principal component* of $p^1(\nu_1), \dots, p^N(\nu_1)$
2. While $\max_{\nu \in \Lambda_{train}} \Delta'(\nu) > \varepsilon$, $X = X + \mathrm{Span}\{\zeta, \zeta'\}$
   ζ *principal component* of $c^1(\bar\nu), \dots, c^N(\bar\nu)$
   ζ' *principal component* of $p^1(\bar\nu), \dots, p^N(\bar\nu)$
   using for $\bar\nu \in \mathrm{argmax}\{\Delta'(\nu), \nu \in \Lambda_{train}\}$

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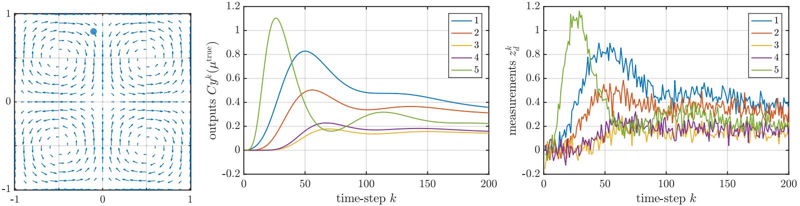
Advection-diffusion in TG vortices

Kärcher M.; Boyaval, S.; Grepl, M. A. & Veroy, K.
Reduced basis approximation and a posteriori error bounds for 4D-Var data assimilation, Optimization and Engineering 2018

advection by: $(\sin(\pi x_1)\cos(\pi x_2), -\cos(\pi x_1)\sin(\pi x_2))$

$\nu \in [.02, .1]$ $\mathbb{P}_1$ $\Delta t = .04$ 200time steps $R \equiv .025$



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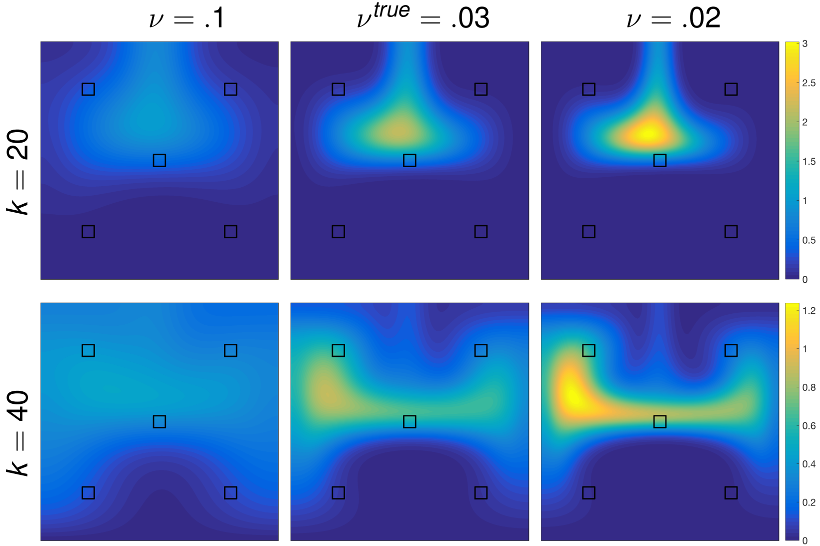

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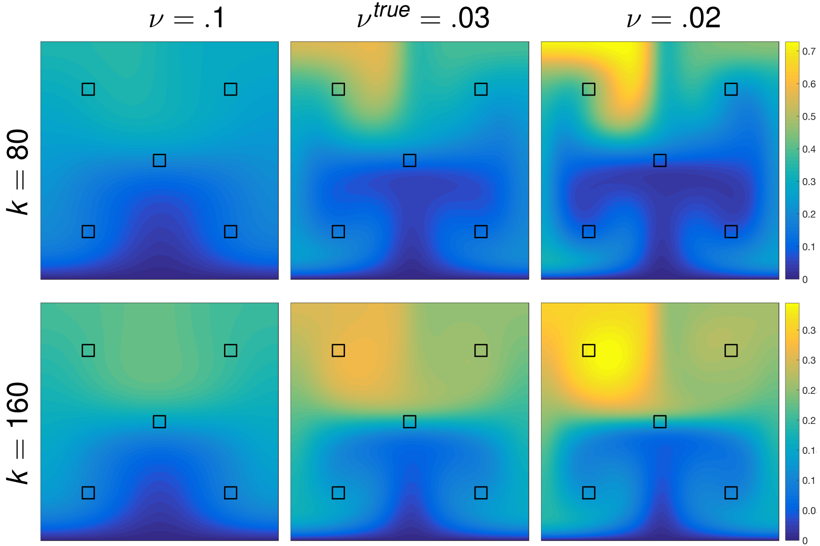
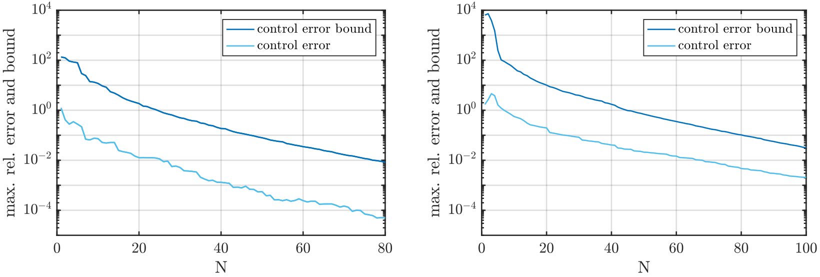


Error estimate

Strong 4DVar $Q = 0$ (left) and weak $Q = .1$ (right)



Optimum: $\nu^* = .034$ (strong), .022 (weak)

N	$e_{J,N}^{\max}$ (strong)	$e_{\nu,N}$ (strong)	$e_{J,N}^{\max}$ (weak)	$e_{\nu,N}$ (weak)
10	3.12e-01	4.18e-01	2.44e-01	6.02e-02
20	7.36e-03	1.30e-01	1.70e-02	9.33e-03
30	8.22e-04	1.42e-03	3.51e-03	1.70e-04
40	1.24e-04	4.99e-04	6.37e-04	3.26e-04
50	1.14e-05	2.98e-05	2.05e-04	3.53e-05
60	4.36e-06	1.27e-05	9.70e-05	3.90e-05
70	3.92e-07	4.18e-06	3.58e-05	1.93e-05
80	8.76e-08	9.71e-08	1.05e-05	4.12e-06
90	-	-	4.17e-06	2.51e-06
100	-	-	1.94e-06	3.09e-06

Conclusion & Perspectives

- RB can be specialized to 4DVar with (LTI) parabolic PDEs
- Other models / DA procedures ?

Thanks for listening