# Sparse grid and reduced basis approximation for Bayesian inverse problems

Peng Chen<sup>1</sup> joint work with Christoph Schwab<sup>1</sup>

Acknowledgement: Alfio Quarteroni<sup>2</sup> Gianluigi Rozza<sup>3</sup>

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Pro\*Doc Retreat Disentis, August 13 - 15, 2014

# Outline

- Bayesian inverse problems
- 2 Sparse grid approximation
- 3 Reduced basis approximation
  - 4 A priori error estimates
- 5 Numerical experiments
- 6 Conclusion and perspective

Problem: given noisy observation data for system output, to calibrate unknown input.

- *X* (separable Banach) space for unknown input ;
- *Y* (separable Banach) space for system output.

Given a forward operator (e.g. PDEs, system of ODEs, etc.)

 $G: X \to Y,$ 

and a observation operator (a set of sensors, e.g. pointwise data, Gaussian average)

 $\mathcal{O}: Y \to \mathbb{R}^K,$ 

with  $K \in \mathbb{N}$ . We define the map from unknown input to finite data

$$\mathcal{G} := \mathcal{O} \circ G : X \to \mathbb{R}^K.$$

The inverse problem: find  $u \in X$  given the noisy observation

$$\boldsymbol{\delta} = \mathcal{G}(\boldsymbol{u}) + \eta,$$

where  $\eta \in \mathbb{R}^{K}$  represents the noise, e.g. drawn from the Gaussian measure  $\mathcal{N}(0,\Gamma)$ .

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# Bayesian inverse problems [Stuart, 2010]

**Bayesian approach**: given data  $\delta$ , to update the distribution of the unknown input *u*.

- Let *u* be a random variable with Lebesgue density  $\rho_0(u)$ ;
- Assume the noise η is independent of u with Lebesgue density ρ(η);
- So  $(u, \delta)$  is a random variable with Lebesgue density  $\rho(\delta \mathcal{G}(u))\rho_0(u)$ .

#### Bayes' theorem

Assume that the probability of  $\delta$  is positive, i.e.

$$Z:=\int_X \rho(\delta-\mathcal{G}(u))\rho_0(u)du>0,$$

Then  $u|\delta$  is a random variable with Lebesgue density  $\rho^{\delta}$  given by

$$\underbrace{\rho^{\delta}(u)}_{\text{osterior density}} = \frac{1}{Z} \underbrace{\rho(\delta - \mathcal{G}(u))}_{\text{likelihood}} \underbrace{\rho_{0}(u)}_{\text{prior density}} .$$
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Given data  $\delta$  and the prior density  $\rho_0(u)$ , to determine the posterior density  $\rho^{\delta}(u)$ .

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Parametric representation of the unknown input *u*.

The input *u* admits parametric representation, e.g. with an affine structure

$$u(y) = \psi_0 + \sum_{j \in \mathbb{J}} y_j \psi_j, \quad \psi_0, \psi_j \in X, \quad y_j \sim \mathcal{U}(-1, 1),$$

being  $\mathbb{J}$  a finite or countably infinite set, i.e.  $\mathbb{J} = \{1, \dots, J\}$  with  $J \in \mathbb{N}$ , or  $\mathbb{J} = \mathbb{N}$ .

**Parametric problem:** let  $\mathcal{X}$  and  $\mathcal{Y}$  be two reflexive Banach spaces with duals  $\mathcal{X}', \mathcal{Y}'$ ; let  $A : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$  denote a bilinear form and  $F : \mathcal{Y} \to \mathbb{R}$  a linear functional; we consider

ind 
$$p(y) \in \mathcal{X}$$
 such that  $A(p(y), v; y) = F(v) \quad \forall v \in \mathcal{Y},$  (2)

where we assume that the bilinear form admits the affine structure

Affine parametrization: 
$$A(w, v; y) = A_0(w, v) + \sum_{j \in \mathbb{J}} y_j A_j(w, v).$$
 (3)

inf-sup condition: 
$$\inf_{0 \neq v \in \mathcal{X}} \sup_{0 \neq v \in \mathcal{Y}} \frac{|A(w, v; y)|}{||w||_{\mathcal{X}} ||v||_{\mathcal{Y}}} = \beta(y).$$

diffusion problem, Stokes flow, linear elasticity, acoustic problem, electromagnetics, etc. **Example:**  $A_j(w, v) = \int_{\Omega} \psi_j(x) \nabla w(x) \cdot \nabla v(x) d(x) \quad \forall w, v \in H_0^1(D), \ j \in \{0\} \cup \mathbb{J}.$  Parametric representation of the unknown input *u*.

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$$A_j(w,v) = \int_D \psi_j(x) \nabla w(x) \cdot \nabla v(x) d(x) \quad \forall w, v \in H^1_0(D), \ j \in \{0\} \cup \mathbb{J}.$$

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Let  $U = [-1, 1]^{\mathbb{J}}$  and  $\mathcal{B}$  be the  $\sigma$ -algebra on U. We equip  $(U, \mathcal{B})$  with the prior measure

$$\mu_0(dy) = \bigotimes_{j \in \mathbb{J}} \frac{dy_j}{2}.$$
 (4)

By Radon–Nikodym theorem, the posterior measure is given by

$$\frac{d\mu^{\delta}}{d\mu_{0}}(y) = \frac{1}{Z}\Theta(y),\tag{5}$$

where

$$\Theta(y) := \rho(\delta - \mathcal{O}(p(y))) \text{ and } Z := \mathbb{E}[\Theta] = \int_{U} \Theta(y) \mu_0(dy).$$
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In the case  $\eta \sim \mathcal{N}(0, \Gamma)$ , we have

$$\Theta(\mathbf{y}) = \frac{1}{\sqrt{(2\pi)^{K}|\Gamma|}} \exp\left(-\frac{1}{2}(\delta - \mathcal{O}(p(\mathbf{y})))^{\top}\Gamma^{-1}(\delta - \mathcal{O}(p(\mathbf{y})))\right).$$

Given the prior measure  $\mu_0$  and the data  $\delta$ , to determine the posterior measure  $\mu^o$ .

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Computational quantities of interests (Qols): 1. pointwise  $\Theta(y)$  and 2. integration Z.

#### Computational requests

- **()** Given any  $y \in U$ , solve the parametric problem (2), and evaluate  $\Theta(y)$  through (6).
- ② Evaluate Z by some integration scheme, e.g. Monte Carlo, Gauss quadrature rule.

#### Computational challenges

- Curse-of-dimensionality: when the dimension |J| of the parameter space becomes very high or infinite, too many (millions or more) solutions are needed, e.g. MC.
- Large-scale computation: one solution is very expensive (taking hours by the fastest supercomputers), so only a few tens or hundreds of them are affordable.

- Sparsity: the dimensions are anisotropic and/or only have low mutual interaction.
- Reducibility: the solution/QoIs live in an intrinsically low-dimensional manifold.

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#### Sparsity: low mutual dimensional interaction and/or anisotropic property



# Sparse grid approximation: univariate hierarchical construction

Let  $\mathcal{I}_q$  denote a univariate interpolation operator given by

$$\mathcal{I}_{q}g = \sum_{k=1}^{m(q)} g(y_{k}^{q}) l_{y_{k}^{q}}(y) \quad \text{vs} \quad \mathcal{I}_{q}g = \sum_{i=1}^{q} \triangle^{i}g \equiv \sum_{i=1}^{q} (\mathcal{I}_{i} - \mathcal{I}_{i-1})g,$$
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where q is grid level, m(q) is # nodes,  $m_{\triangle}^{i}$  is index set for additional nodes at level i.



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# Sparse grid approximation: Smolyak sparse grid [Smolyak, 1963]



Hierarchical construction of Smolyak sparse grid.

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SG & RB for Bayesian Inverse Problems

# Sparse grid approximation: adaptive SG [Gerstner and Griebel, 2003]



**Admissible**: if  $i \in \Lambda_M$  then  $i - e_i \in \Lambda_M$  for any  $j \in J$ . X XX XX XXX XXXX XXXX XXX  $\times \times \times \boxtimes$ XXXX XXXXX XXXX ×××× XXXXXX XXXXXX XXXXXXXX XXXX XXXXXX \*\*\*\*\* XXXX XXXXXX XXXXXXXXX XXXXX \*\*\*\*\* ××××××××××× XXXXXXXX XXXXXX \*\*\*\*\* XXXX XXXXXX XXXXXXX

Admissible set of indices for dimension adaptive sparse grid construction. Colored square: active index set  $\mathscr{A}$ ; red square: the index to process in next step.

1 2 3

7 8 9 10 11 12 13 14

$$S_{\Lambda_M}g(y) = \sum_{i \in \Lambda_M} \sum_{k \in m_\Delta^i} \underbrace{\left(g(y_k^i) - S_{\Lambda_M \setminus \{i\}}g(y_k^i)\right)}_{s_k^i} t_k^i(y). \tag{9}$$
$$\mathbb{E}[g] \approx \mathbb{E}[S_{\Lambda_M}g] = \sum_{i \in \Lambda_M} \sum_{k \in m_\Delta^i} s_k^i \mathbb{E}[t_k^i] = \sum_{i \in \Lambda_M} \sum_{k \in m_\Delta^i} s_k^i w_k^i. \tag{10}$$

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# Sparse grid approximation: adaptive SG [Gerstner and Griebel, 2003]



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1 2 3 4 5

#### Interpolation error indicator

$$i = \operatorname*{argmax}_{i' \in \mathscr{A}} \mathcal{E}_i(i'), ext{ with } \mathcal{E}_i(i') = rac{1}{|m_{\bigtriangleup}^{i'}|} \sum_{k \in m_{\bigtriangleup}^{i'}} |s_k^{i'}|.$$

#### Integration error indicator

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#### Interpolation and integration error estimators

$$\mathcal{E}_i(\mathscr{A}) = \max_{i \in \mathscr{A}} \max_{k \in m_{\Delta}^i} |s_k^i| \text{ and } \mathcal{E}_e(\mathscr{A}) = \left| \sum_{i \in \mathscr{A}} \sum_{k \in m_{\Delta}^i} s_k^i w_k^i \right|.$$

Verification algorithm for stagnation problem [Chen and Quarteroni, 2014].

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$$\boldsymbol{i} = \operatorname*{argmax}_{\boldsymbol{i}' \in \mathscr{A}} \mathcal{E}_{e}(\boldsymbol{i}'), ext{ with } \mathcal{E}_{e}(\boldsymbol{i}') = rac{1}{|m_{\bigtriangleup}^{i'}|} \left| \sum_{k \in m_{\bigtriangleup}^{i'}} s_{k}^{i} w_{k}^{i'} \right|.$$

### Interpolation and integration error estimators

$$\mathcal{E}_i(\mathscr{A}) = \max_{i \in \mathscr{A}} \max_{k \in m_{\Delta}^i} |s_k^i| \text{ and } \mathcal{E}_e(\mathscr{A}) = \left| \sum_{i \in \mathscr{A}} \sum_{k \in m_{\Delta}^i} s_k^i w_k^i \right|$$

Verification algorithm for stagnation problem [Chen and Quarteroni, 2014]

Peng Chen (ETH Zurich)

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### High-fidelity approximation: large-scale computation

- High-fidelity approximation spaces:  $X_h \subset X$  and  $Y_h \subset Y$ ;
- Let  $(w_h^n)_{n=1}^{\mathcal{N}}$  and  $(v_h^n)_{n=1}^{\mathcal{N}}$  denote the bases of  $\mathcal{X}_h$  and  $\mathcal{Y}_h$ ;

The high-fidelity solution  $p_h(y)$  can be expanded on the bases  $(w_h^n)_{n=1}^N$  as

$$p_{h}(y) = \sum_{n=1}^{N} p_{h}^{n}(y) w_{h}^{n}, \qquad (11)$$

with  $\mathbf{p}_h(y) = (p_h^1(y), \dots, p_h^{\mathcal{N}}(y))^{\top}$ . The high-fidelity (Petrov)-Galerkin approximation given any  $y \in U$ , find  $p_h(y) \in \mathcal{X}_h$  such that  $A(p_h(y), v_h; y) = F(v_h) \quad \forall v_h \in \mathcal{Y}_h$ . (12)

Let 
$$(\mathbb{A}_h^j)_{nn'} := A_j(w_h^n, v_h^{n'}) \ 1 \le n, n' \le \mathcal{N}, \mathbf{f}_h = (F(v_h^1), \dots, F(v_h^{\mathcal{N}}))^\top$$
, then

given any 
$$y \in U$$
, find  $\mathbf{p}_h(y) \in \mathbb{R}^N$  such that  $\left(\mathbb{A}_h^0 + \sum_{j \in \mathbb{J}} y_j \mathbb{A}_h^j\right) \mathbf{p}_h(y) = \mathbf{f}_h$ , (13)

which is a  $\mathcal{N} \times \mathcal{N}$  system, requiring large-scale computation when  $\mathcal{N}$  is very large.

### High-fidelity approximation: large-scale computation

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Let  $(\mathbb{A}_{h}^{j})_{nn'} := A_{j}(w_{h}^{n}, v_{h}^{n'}) \ 1 \le n, n' \le \mathcal{N}, \ \mathbf{f}_{h} = (F(v_{h}^{1}), \dots, F(v_{h}^{\mathcal{N}}))^{\top}, \ \text{then}$ 

given any 
$$y \in U$$
, find  $\mathbf{p}_h(y) \in \mathbb{R}^{\mathcal{N}}$  such that  $\left(\mathbb{A}_h^0 + \sum_{j \in \mathbb{J}} y_j \mathbb{A}_h^j\right) \mathbf{p}_h(y) = \mathbf{f}_h$ , (13)

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# Reduced basis approximation: low-dimensional manifold

**Reducibility:** the solution manifold  $\mathcal{M} = \{p_h(y) \in \mathcal{X}_h, y \in U\}$  is low-dimensional.



Mathematically, the best approximation error decays very fast

Kolmogorov *N*-width:  $d_N(\mathcal{X}_h, \mathcal{M}) := \inf_{\mathcal{Z}_N \subset \mathcal{X}_h} \sup_{v \in \mathcal{A}_N} \inf_{w \in \mathcal{Z}_N} ||v - w||_{\mathcal{X}} \equiv \inf_{\mathcal{Z}_N \subset \mathcal{X}_h} \mathsf{dist}(\mathcal{Z}_N, \mathcal{M}).$ 

Look for a low-dimensional reduced basis space  $\mathcal{X}_N \subset \mathcal{M}$  such that

reduced basis error: 
$$\sigma_N(\mathcal{X}_N, \mathcal{M}) := \sup_{v \in \mathcal{M}} \inf_{w \in \mathcal{X}_N} ||v - w||_{\mathcal{X}} \equiv \operatorname{dist}(\mathcal{X}_N, \mathcal{M}),$$

converges with rate not far from (ideally achieves) that of the best approximation error.

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Look for a low-dimensional reduced basis space  $\mathcal{X}_{\scriptscriptstyle N} \subset \mathcal{M}$  such that

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$$\sigma_N(\mathcal{X}_N, \mathcal{M}) := \sup_{v \in \mathcal{M}} \inf_{w \in \mathcal{X}_N} ||v - w||_{\mathcal{X}} \equiv \mathsf{dist}(\mathcal{X}_N, \mathcal{M}),$$

converges with rate not far from (ideally achieves) that of the best approximation error.
## Reduced basis approximation: reduction [Patera and Rozza, 2007]

- Reduced basis approximation spaces: X<sub>N</sub> ⊂ X<sub>h</sub> and Y<sub>N</sub> ⊂ Y<sub>h</sub>;
- Let  $(w_N^n)_{n=1}^N$  and  $(v_N^n)_{n=1}^N$  denote the bases of  $\mathcal{X}_N$  and  $\mathcal{Y}_N$ ;

The reduced solution  $p_h(y)$  can be expanded on the bases  $(w_N^n)_{n=1}^N$  as

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with  $\mathbf{p}_N(y) = (p_N^1(y), \dots, p_N^N(y))^\top$ . The reduced basis (Petrov)-Galerkin approximation given any  $y \in U$ , find  $p_N(y) \in \mathcal{X}_N$  such that  $A(p_N(y), v_N; y) = F(v_N) \quad \forall v_N \in \mathcal{Y}_N$ . (15)

Let 
$$\mathbb{W} = (\mathbf{w}_N^1, \dots, \mathbf{w}_N^N)$$
 and  $\mathbb{V} = (\mathbf{v}_N^1, \dots, \mathbf{v}_N^N)$ ,  $\mathbb{A}_N^j = \mathbb{V}^\top \mathbb{A}_h^j \mathbb{W}$ ,  $j \in \{0\} \cup \mathbb{J}$ ;  $\mathbf{f}_N = \mathbb{V}^\top \mathbf{f}_h$ .

given any 
$$y \in U$$
, find  $\mathbf{p}_N(y) \in \mathbb{R}^N$  such that  $\left(\mathbb{A}_N^0 + \sum_{j \in \mathbb{J}} \mathbf{y}_j \mathbb{A}_N^j\right) \mathbf{p}_N(y) = \mathbf{f}_N.$  (16)

which is a  $N \times N$  system, needs small-scale computation as  $N \ll N$ , e.g.  $(10 \sim 100)$ .

- Reduced basis approximation spaces:  $\mathcal{X}_N \subset \mathcal{X}_h$  and  $\mathcal{Y}_N \subset \mathcal{Y}_h$ ;
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# Reduced basis approximation: construction of reduced spaces

#### Greedy algorithm [Patera and Rozza, 2007]

Initialize  $\mathcal{X}_1 = \text{span}\{p_h(y^{(1)})\}$  at some random sample  $y^{(1)}$ , then for N = 2, 3, ...,

$$y^{(N)} = \underset{y \in U}{\operatorname{argsup}} ||p_h(y) - p_{N-1}(y)||_{\mathcal{X}} \quad \text{or} \quad y^{(N)} = \underset{y \in U}{\operatorname{argsup}} |\Theta_h(y) - \Theta_{N-1}(y)|$$
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and the reduced space  $\mathcal{X}_N$  can be constructed by the snapshots

$$\mathcal{X}_N = \mathcal{X}_{N-1} \oplus \operatorname{span}\{p_h(y^{(N)})\}.$$
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Gram–Schmidt process  $\rightarrow$  orthnormal bases  $(w_N^n)_{n=1}^N$  of  $\mathcal{X}_N$  for better stability of  $\mathbb{A}_N(y)$ .

- In case of symmetric coercive *A*, we can directly take  $\mathcal{Y}_N = \mathcal{X}_N$ ;
- otherwise, we solve a 'supremizer' problem (to guarantee the inf-sup condition)

given  $y \in U$ , find  $v_N^n(y) \in \mathcal{Y}_h$  such that  $(v_N^n(y), v_h)_{\mathcal{Y}_h} = A(w_N^n, v_h; y) \quad \forall v_h \in \mathcal{Y}_h$ , (19) Let  $\mathbb{A}_N^{j,j'} = (\mathbb{A}_h^j \mathbb{W})^\top \mathbb{M}_h^{-1} \mathbb{A}_h^{j'} \mathbb{W}$ , and  $\mathbf{f}_N^j = (\mathbb{A}_h^j \mathbb{W})^\top \mathbb{M}_h^{-1} \mathbf{f}_h$ ; we solve the  $N \times N$  system  $\left(\mathbb{A}_N^{0,0} + 2\sum_{j \in \mathbb{J}} y_j \mathbb{A}_N^{0,j} + \sum_{j \in \mathbb{J}} \sum_{j' \in \mathbb{J}} y_j y_{j'} \mathbb{A}_N^{j,j'}\right) \mathbf{p}_N(y) = \mathbf{f}_N^0 + \sum_{j \in \mathbb{J}} y_j \mathbf{f}_N^j.$  (20)

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$$\mathbb{A}_{N}^{0,0} + 2\sum_{j\in\mathbb{J}} y_{j}\mathbb{A}_{N}^{0,j} + \sum_{j\in\mathbb{J}} \sum_{j'\in\mathbb{J}} y_{j}y_{j'}\mathbb{A}_{N}^{j,j'} \right) \mathbf{p}_{N}(y) = \mathbf{f}_{N}^{0} + \sum_{j\in\mathbb{J}} y_{j}\mathbf{f}_{N}^{j}.$$
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# Reduced basis approximation: a posteriori error estimators I

We consider the error estimator for the nonlinear, nonaffine Qol. Recall by definition

$$\Theta_{h}(\mathbf{y}) = \frac{1}{\sqrt{(2\pi)^{K}|\Gamma|}} \exp\left(-\frac{1}{2}(\delta - \mathcal{O}(p_{h}(\mathbf{y})))^{\top}\Gamma^{-1}(\delta - \mathcal{O}(p_{h}(\mathbf{y})))\right),$$

which can be expanded as

$$\Theta_h(y) = \Theta_N(y) + \frac{\partial \Theta_h}{\partial p_h} \Big|_{p_N(y)} (p_h(y) - p_N(y)) + O(||p_h(y) - p_N(y)||_{\mathcal{X}}^2).$$
(21)

We can estimate the error by

$$|\Theta_h(y) - \Theta_N(y)| \approx \left| \frac{\partial \Theta_h}{\partial p_h} \right|_{p_N(y)} (p_h(y) - p_N(y)) \right| \leq \left| \left| \frac{\partial \Theta_h}{\partial p_h} \right|_{p_N(y)} \right| \Big|_{\mathcal{X}'} ||p_h(y) - p_N(y)||_{\mathcal{X}} =: \Delta_N^{(1)}(y).$$

Here, the reduced solution error can be bounded by

$$||p_h(y) - p_N(y)||_{\mathcal{X}} \leq \frac{||R_h(\cdot; y)||_{\mathcal{Y}'}}{\beta_h(y)} =: \triangle_N^p(y),$$

where the residual  $R_h(\cdot; y) \in \mathcal{Y}'$ , defined as

$$R_h(v_h; y) = F(v_h) - A(p_N(y), v_h; y) \quad \forall v_h \in \mathcal{Y}_h,$$

and the inf-sup constant  $eta_h(y)$  is uniformly bounded from below by  $eta_h^{LB}$ 

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and the inf-sup constant  $\beta_h(y)$  is uniformly bounded from below by  $\beta_h^{LB}$ .

## Reduced basis approximation: a posteriori error estimators II

We consider a dual problem corresponding to the primal problem (12) reads as

given any 
$$y \in U$$
, find  $\psi_h(y) \in \mathcal{Y}_h$  such that  $A(w_h, \psi_h; y) = \frac{\partial \Theta_h}{\partial p_h}\Big|_{p_N(y)}(w_h) \quad \forall w_h \in \mathcal{X}_h.$ 

We may approximate this high-fidelity solution with a reduced dual solution by solving

find 
$$\psi_{N_{du}}(y) \in \mathcal{Y}_{N_{du}}$$
 such that  $A(w_{N_{du}}^{du}, \psi_{N_{du}}; y) = \frac{\partial \Theta_h}{\partial p_h}\Big|_{p_N(y)}(w_{N_{du}}^{du}) \quad \forall w_{N_{du}}^{du} \in \mathcal{X}_{N_{du}}.$  (22)

The second error estimator (dual-weighted residual) is simply defined as

$$\Delta_{N}^{(2)}(\mathbf{y}) := R(\psi_{N_{du}}(\mathbf{y}); \mathbf{y}) = \mathbf{f}_{h}^{\top} \mathbb{W}_{du} \boldsymbol{\psi}_{N_{du}}(\mathbf{y}) - \sum_{j \in \{0\} \cup \mathbb{J}} y_{j}(\mathbf{p}_{N}(\mathbf{y}))^{\top} \mathbb{W}^{\top} \mathbb{A}_{h}^{j} \mathbb{W}_{du} \boldsymbol{\psi}_{N_{du}}(\mathbf{y})$$
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A closer look at the residual (by Galerkin orthogonality):

$$R(\psi_h(y); y) = A(p_h(y) - p_N(y), \psi_h(y); y) = \frac{\partial \Theta_h}{\partial p_h} \Big|_{p_N(y)} (p_h(y) - p_N(y)),$$
(24)

which is nothing but the first term in the expansion. Moreover,

$$R(\psi_h(y); y) - \triangle_N^{(2)}(y) = R(e_h^{du}(y); y) = A(e_h(y), e_h^{du}(y); y) \le \gamma_h(y) ||e_h(y)||_{\mathcal{X}} ||e_h^{du}(y)||_{\mathcal{Y}},$$
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where we denote the reduced errors  $e_h(y) = p_h(y) - p_N(y)$  and  $e_h^{du}(y) = \psi_h(y) - \psi_{N_{du}}(y)$ .

## Reduced basis approximation: a posteriori error estimators II

We consider a dual problem corresponding to the primal problem (12) reads as

given any  $y \in U$ , find  $\psi_h(y) \in \mathcal{Y}_h$  such that  $A(w_h, \psi_h; y) = \frac{\partial \Theta_h}{\partial p_h}\Big|_{p_N(y)}(w_h) \quad \forall w_h \in \mathcal{X}_h.$ 

We may approximate this high-fidelity solution with a reduced dual solution by solving

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$$\psi_{N_{du}}(y) \in \mathcal{Y}_{N_{du}}$$
 such that  $A(w_{N_{du}}^{du}, \psi_{N_{du}}; y) = \frac{\partial \Theta_h}{\partial p_h}\Big|_{p_N(y)}(w_{N_{du}}^{du}) \quad \forall w_{N_{du}}^{du} \in \mathcal{X}_{N_{du}}.$  (22)

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$$\Delta_N^{(2)}(\mathbf{y}) := R(\psi_{N_{du}}(\mathbf{y}); \mathbf{y}) = \mathbf{f}_h^\top \mathbb{W}_{du} \boldsymbol{\psi}_{N_{du}}(\mathbf{y}) - \sum_{j \in \{0\} \cup \mathbb{J}} y_j(\mathbf{p}_N(\mathbf{y}))^\top \mathbb{W}^\top \mathbb{A}_h^j \mathbb{W}_{du} \boldsymbol{\psi}_{N_{du}}(\mathbf{y})$$
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# Reduced basis approximation: a posteriori error estimators III

#### We may propose the use of a (improved/corrected) reduced output

$$\Theta_N^c(y) = \Theta_N(y) + \Delta_N^{(2)}(y).$$
(26)

The last term in the expansion can be further expanded as

$$O(||p_h(y) - p_N(y)||_{\mathcal{X}}^2) = \frac{1}{2} \frac{\partial^2 \Theta_h}{\partial p_h^2} \Big|_{p_N(y)} (p_h(y) - p_N(y), p_h(y) - p_N(y)) + O(||p_h(y) - p_N(y)||_{\mathcal{X}}^3).$$

So that the third a posteriori error estimator can be given by

$$\Delta_N^{(3)}(y) := \max\left\{\Delta_N^{(4)}(y), \Delta_N^{(5)}(y)\right\},\tag{27}$$

where (note  $|\Theta_h(y) - \Theta_N^c(y)| pprox ($  first term  $- riangle_N^{(2)}) +$  second term )

$$\Delta_N^{(4)}(y) := \gamma_h(y) ||e_h(y)||_{\mathcal{X}} ||e_h^{du}(y)||_{\mathcal{Y}}, \text{ and } \Delta_N^{(5)}(y) := \gamma'_h(y) ||e_h(y)||_{\mathcal{X}}^2.$$
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Note that  $\Delta_N^{(4)}$  and  $\Delta_N^{(5)}$  exhibit a **quadratic** dependence on the reduced solution error.

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#### Adaptive greedy algorithm [Chen and Quarteroni, 2014]

**Initialization:** specify tolerance  $\epsilon_t$ , set N = 1, solve the high-fidelity problem at  $y_1^1$ , the root node in the sparse grid, and construct the first reduced space  $\mathcal{X}_1 = \text{span}\{p_h(y_1^1)\}$ ; **While** sparse grid construction continues

at each new index *i*, update the training set  $\Xi_{train} = \Xi_{\Delta}^{i}$ ;

 $\begin{aligned} \lim \max_{y \in \Xi_{train}} \Delta_N(y) &\geq \epsilon_t \\ \text{update } \Xi_{train} \text{ as } \Xi_{train} = \Xi_{train} \setminus \{ y \in \Xi_{train} : \Delta_N(y) < \epsilon_t \} \\ \text{set } y^{(N+1)} = \operatornamewithlimits{argmax}_{A \in Y} \Delta_N(y). \end{aligned}$ 

solve high-fidelity problem at  $y^{(N+1)}$  to obtain  $p_h(y^{(N+1)})$ ;

update  $\mathcal{X}_{N+1} = \mathcal{X}_N \oplus \operatorname{span}\{p_h(y^{(N+1)})\};$ 

set N = N + 1

en

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at each new index i, update the training set \Xi_{main} = \Xi_{\Delta}^i;

While more approximate a span \{p_h(y_1^{(n)})\};

Solve high fidelity problem at y_1^{(n)} to obtain p_h(y_1^{(n)});

update then solve span \{p_h(y_1^{(n)})\};

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## Assumption [Schwab and Stuart, 2012]

There exist  $0 < a_{\min} \le a_{\max} < \infty$ , such that  $\forall z \in \mathcal{U} := \bigotimes_{i \in \mathbb{J}} \{z \in \mathbb{C}^{\mathbb{J}} : |z_i| \le 1\}$ 

$$a_{\min} \le \Re(u(x,z)) \le |u(x,z)| \le a_{\max}, \quad \forall x \in D$$
 (29)

There exists a constant  $0 < \alpha < 1$ , such that (recall  $u(y) = \psi_0 + \sum_{i \in \mathbb{I}} y_i \psi_i$ )

$$\sum_{j\in\mathbb{J}}||\psi_j||^{\alpha}_{L^{\infty}(D)}<\infty. \tag{30}$$

$$\Theta(y) = \underbrace{\Theta(y) - \Theta_s(y)}_{(y) \to (y)} + \underbrace{\Theta_s(y) - \Theta_{s,h}(y)}_{(y) \to (y)} + \underbrace{\Theta_{s,h}(y) - \Theta_{s,h,r}(y)}_{(y) \to (y)} + \underbrace{\Theta_{s,h,r}(y)}_{(y) \to (y)} + \underbrace{\Theta_{s,h,r}(y)}_{(y) \to (y)} + \underbrace{\Theta_{s,h}(y) - \Theta_{s,h,r}(y)}_{(y) \to (y)} + \underbrace{\Theta_{s,h}(y) - \Theta_$$

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#### Global approximation

and

The Qol  $\Theta(y)$  and Z are approximated by

$$\Theta(y) = \underbrace{\Theta(y) - \Theta_{s}(y)}_{\text{interpolation error}} + \underbrace{\Theta_{s}(y) - \Theta_{s,h}(y)}_{\text{high-fidelity error}} + \underbrace{\Theta_{s,h}(y) - \Theta_{s,h,r}(y)}_{\text{reduced basis error}} + \Theta_{s,h,r}(y),$$

$$Z = \underbrace{Z - Z_{s}}_{\text{quadrature error}} + \underbrace{Z_{s} - Z_{s,h}}_{\text{high-fidelity error}} + \underbrace{Z_{s,h} - Z_{s,h,r}}_{\text{reduced basis error}} + Z_{s,h,r}.$$

Peng Chen (ETH Zurich)

$$|\Theta(y) - \Theta_s(y)| \le CM^{-s}$$
 and  $|Z - Z_s| \le CM^{-s}$ ,  $s = \frac{1}{\alpha} - 1$ .

High-fidelity approximation error

$$|\Theta_s(y) - \Theta_{s,h}(y)| \le Ch^t \text{ and } |Z_s - Z_{s,h}| \le Ch^t, \quad t = \min\{t_{polynomial}, t_{regularity}\}.$$

RB approximation error [Binev et al., 2011, Cohen and DeVore, 2014]

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#### Global approximation error

$$\Theta(y) - \Theta_{s,h,r}(y) \le C_0 M^{-s} + C_1 h^t + C_2 N^{-s}.$$

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## Numerical experiments: sparse grid approximation error

We consider a diffusion problem with K = 9 observations. We take  $\mathbb{J} = \{1, \ldots, 64\}$  and  $\psi_0 = 1$  and  $\psi_j = 0.95j^{-2}\chi_{D_j}$ ,  $j \in \mathbb{J}$ , so  $\alpha > 1/2$  and the rate  $-s = -(1/\alpha - 1) > -1$ .



Figure: Interpolation error estimator of the dimension-adaptive sparse grid approximation constructed by the interpolation error indicator (left) and the integration error indicator (right).

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Figure: Integration error estimator of the dimension-adaptive sparse grid approximation constructed by the interpolation error indicator (left) and the integration error indicator (right).



Figure: Left: decay of finite element error with respect to the mesh size (1/h); right: change of the number of reduced bases (constructed with tolerance  $10^{-7}$ ) with respect to the mesh size (1/h).

## Numerical experiments: effectivity of different error estimators



Figure: Left: effectivity of the three error estimators; right: the true reduced output error (truncated above  $10^{-14}$ ) and the effectivity of the dual-weighted residual with respect to this error.

## Numerical experiments: effectivity of different error estimators



Figure: Left: effect of correction  $E_2/E_1$  with  $E_2 = |\Theta_h(y) - \Theta_N^c(y)|$  and  $E_1 = |\Theta_h(y) - \Theta_N(y)|$ ; right: effectivity of  $\triangle_N^{(4)}$  and  $\triangle_N^{(5)}$  defined in (28) with respect to the corrected output error.

## Numerical experiments: reduced basis approximation error

Relative output error without dual correction



Figure: Decay of reduced basis approximation error with respect to the number reduced bases; left: 64 dimensions, fitted rates for the first 32 bases and the other 68 bases; right: 256 D.

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Relative output error with dual correction



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## Conclusion

## • Curse-of-dimensionality can be broken by sparsity – adaptive sparse grid.

- Large-scale computation can be harnessed by reducibility reduced basis.
- Goal-oriented error estimator (dual-weighted residual) achieves **excellent** effectivity for the nonlinear and nonaffine output in Bayesian inverse problems.
- The adaptive sparse grid approximation error and **particularly the reduced basis** approximation error **converges faster** in practice than predicted by theory.

#### Perspective

- Work on the improvement of the theoretical estimate for faster convergence.
- Sparse grid reduced basis approximation for nonlinear and nonaffine problems.
- RB can be efficiently combined with any other quadrature rule, e.g. QMC.
- A global framework for adaptive approximation in balancing all the errors.

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## Conclusion

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# Thank you for your attention!