## Sparse grid and reduced basis approximation for Bayesian inverse problems

Peng Chen ${ }^{1}$<br>joint work with<br>Christoph Schwab ${ }^{1}$

Acknowledgement: Alfio Quarteroni ${ }^{2}$ Gianluigi Rozza ${ }^{3}$

${ }^{1}$ SAM - D-MATH - ETH, Zurich<br>${ }^{2}$ CMCS - MATHICSE - EPFL, Lausanne

${ }^{3}$ MathLab - SISSA - International School for Advanced Studies, Trieste, Italy

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## Outline

(1) Bayesian inverse problems
(2) Sparse grid approximation
(3) Reduced basis approximation

4 A priori error estimates
(5) Numerical experiments
(6) Conclusion and perspective

## Bayesian inverse problems [Stuart, 2010]

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.)

and a observation operator (a set of sensors, e.g. pointwise data, Gaussian average)
with $K \in \mathbb{N}$. We define the map from unknown input to finite data


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G: X \rightarrow Y,
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\mathcal{O}: Y \rightarrow \mathbb{R}^{K}
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$$
\delta=\mathcal{G}(u)+\eta,
$$

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

## 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 $\eta$ is independent of $u$ with Lebesgue density $\rho(\eta)$;
- 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.

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


Given data $\delta$ and the prior density $\rho_{0}(u)$, to determine the posterior density $\rho^{\delta}(u)$.

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Z:=\int_{X} \rho(\delta-\mathcal{G}(u)) \rho_{0}(u) d u>0,
$$

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

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

## Bayesian inverse problems: parametrization [Schwab and Stuart, 2012]

## 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. $\mathbb{J}=\{1, \ldots, J\}$ 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 $\mathcal{X}^{\prime}, \mathcal{Y}^{\prime} ;$
let $A: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$ denote a bilinear form and $F: \mathcal{Y} \rightarrow \mathbb{R}$ a linear functional; we consider find $p(y) \in \mathcal{X}$ such that $\quad A(p(y), v ; y)=F(v) \quad \forall v \in \mathcal{Y}$
where we assume that the bilinear form admits the affine structure Affine parametrization:
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diffusion problem, Stokes flow, linear clasticity, acoustic problem, electromagnetics, etc.

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\text { find } p(y) \in \mathcal{X} \text { such that } \quad A(p(y), v ; y)=F(v) \quad \forall v \in \mathcal{Y}, \tag{2}
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where we assume that the bilinear form admits the affine structure
Affine parametrization: $A(w, v ; y)=A_{0}(w, v)+\sum_{j \in \mathbb{J}} y_{j} A_{j}(w, v)$.

$$
\text { inf-sup condition: } \inf _{0 \neq w \in \mathcal{X}} \sup _{0 \neq v \in \mathcal{Y}} \frac{|A(w, v ; y)|}{\|w\| \mathcal{X}\|v\|_{\mathcal{Y}}}=\beta(y) .
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Example: $\quad A_{j}(w, v)=\int_{D} \psi_{j}(x) \nabla w(x) \cdot \nabla v(x) d(x) \quad \forall w, v \in H_{0}^{1}(D), j \in\{0\} \cup \mathbb{J}$.

## Bayesian inverse problems: parametrization [Schwab and Stuart, 2012]

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

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\begin{equation*}
\mu_{0}(d y)=\bigotimes_{j \in \mathbb{J}} \frac{d y_{j}}{2} \tag{4}
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## By Radon-Nikodym theorem, the posterior measure is given by



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\begin{equation*}
\Theta(y):=\rho(\delta-\mathcal{O}(p(y))) \text { and } Z:=\mathbb{E}[\Theta]=\int_{U} \Theta(y) \mu_{0}(d y) \tag{6}
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In the case $\eta \sim \mathcal{N}(0, \Gamma)$, we have


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In the case $\eta \sim \mathcal{N}(0, \Gamma)$, we have

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\Theta(y)=\frac{1}{\sqrt{(2 \pi)^{K}|\Gamma|}} \exp \left(-\frac{1}{2}(\delta-\mathcal{O}(p(y)))^{\top} \Gamma^{-1}(\delta-\mathcal{O}(p(y)))\right) .
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## Bayesian inverse problems: computational aspects

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).
© Evaluate Z by some integration scheme, e.g. Monte Carlo, Gauss quadrature rule.
omputational 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.


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


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## Sparse grid approximation: a first look (see also Robert's talk)

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

$$
\begin{equation*}
\mathcal{I}_{q} g=\sum_{k=1}^{m(q)} g\left(y_{k}^{q}\right) l_{y_{k}^{g}}(y) \quad \text { vs } \quad \mathcal{I}_{q} g=\sum_{i=1}^{q} \Delta^{i} g \equiv \sum_{i=1}^{q}\left(\mathcal{I}_{i}-\mathcal{I}_{i-1}\right) g, \tag{7}
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## Sparse grid approximation: Smolyak sparse grid [Smolyak, 1963]

$$
\begin{gathered}
\mathcal{S}_{q} g=\sum_{|i| \leq q}\left(\triangle_{1}^{i_{1}} \otimes \cdots \otimes \triangle_{J}^{i_{J}}\right) g=\sum_{|i|=J}^{q} \triangle \mathcal{S}_{|i|} g(y) \\
\triangle \mathcal{S}_{q} g(y)=\sum_{|i|=q} \sum_{k \in m^{i}} \underbrace{\left(g\left(y_{k_{1}}^{i_{1}}, \ldots, y_{k_{J}}^{i_{J}}\right)-\mathcal{S}_{q-1} g\left(y_{k_{1}}^{i_{1}}, \ldots, y_{k_{J}}^{i_{J}}\right)\right)}_{s_{k}^{i}} \underbrace{\left(l_{k_{1}}^{i_{1}}\left(y_{1}\right) \otimes \cdots \otimes l_{k_{J}}^{i_{J}}\left(y_{J}\right)\right)}_{i_{k}^{i}} .
\end{gathered}
$$



Hierarchical construction of Smolyak sparse grid.

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

$$
\Lambda_{s}=\left\{\boldsymbol{i} \in \mathbb{N}_{+}^{K}:|\boldsymbol{i}| \leq q\right\} \rightarrow \Lambda_{M}=\left\{\boldsymbol{i} \in \mathbb{N}_{+}^{K}: \boldsymbol{i} \text { admissible }\right\} .
$$

Admissible: if $\boldsymbol{i} \in \Lambda_{M}$ then $\boldsymbol{i}-e_{j} \in \Lambda_{M}$ for any $j \in \mathbb{J}$.


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.

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\begin{align*}
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& \mathbb{E}[g] \approx \mathbb{E}\left[\mathcal{S}_{\Lambda_{M}} g\right]=\sum_{i \in \Lambda_{M}} \sum_{k \in m_{\Delta}^{i}} s_{k}^{i} \mathbb{E}\left[l_{k}^{i}\right]=\sum_{i \in \Lambda_{M}} \sum_{k \in m_{\Delta}^{i}} s_{k}^{i} w_{k}^{i} . \tag{10}
\end{align*}
$$

## Sparse grid approximation: error indicators and estimators

## Interpolation error indicator

$$
i=\underset{i^{\prime} \in \mathscr{A}}{\operatorname{argmax}} \mathcal{E}_{i}\left(\boldsymbol{i}^{\prime}\right), \text { with } \mathcal{E}_{i}\left(\boldsymbol{i}^{\prime}\right)=\frac{1}{\left|m_{\triangle}^{i^{\prime}}\right|} \sum_{k \in m_{\triangle}^{i^{\prime}}}\left|s_{\boldsymbol{k}}^{i^{\prime}}\right|
$$

## Integration error indicator

## Interpolation and integration error estimators

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

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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}}\left|s_{k}^{i}\right| \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| .
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## Verification algorithm for stagnation problem [Chen and Quarteroni, 2014].

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## Interpolation and integration error estimators

$$
\mathcal{E}_{i}(\mathscr{A})=\max _{i \in \mathscr{A}} \max _{k \in m_{\triangle}^{i}}\left|s_{k}^{i}\right| \text { and } \mathcal{E}_{e}(\mathscr{A})=\left|\sum_{i \in \mathscr{A}} \sum_{k \in m_{\Delta}^{i}} s_{k}^{i} w_{k}^{i}\right| .
$$

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

## High-fidelity approximation: large-scale computation

- High-fidelity approximation spaces: $\mathcal{X}_{h} \subset \mathcal{X}$ and $\mathcal{Y}_{h} \subset \mathcal{Y}$;
- Let $\left(w_{h}^{n}\right)_{n=1}^{\mathcal{N}}$ and $\left(v_{h}^{n}\right)_{n=1}^{\mathcal{N}}$ denote the bases of $\mathcal{X}_{h}$ and $\mathcal{Y}_{h}$;

given any $y \in U$, find $p_{h}(y) \in \mathcal{X}_{h}$ such that $A\left(p_{h}(y), v_{h} ; y\right)=F\left(v_{h}\right) \quad \forall v_{h} \in \mathcal{Y}_{h}$.

Let $\left(\mathbb{A}_{h}^{j}\right)_{n n^{\prime}}:=A_{j}\left(w_{h}^{n}, v_{h}^{n^{\prime}}\right) 1 \leq n, n^{\prime} \leq \mathcal{N}, \mathbf{f}_{h}=\left(F\left(v_{h}^{1}\right), \ldots, F\left(v_{h}^{\mathcal{N}}\right)\right)^{\top}$, then


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- Let $\left(w_{h}^{n}\right)_{n=1}^{\mathcal{N}}$ and $\left(v_{h}^{n}\right)_{n=1}^{\mathcal{N}}$ denote the bases of $\mathcal{X}_{h}$ and $\mathcal{Y}_{h}$;

The high-fidelity solution $p_{h}(y)$ can be expanded on the bases $\left(w_{h}^{n}\right)_{n=1}^{\mathcal{N}}$ as

$$
\begin{equation*}
p_{h}(y)=\sum_{n=1}^{\mathcal{N}} p_{h}^{n}(y) w_{h}^{n}, \tag{11}
\end{equation*}
$$

with $\mathbf{p}_{h}(y)=\left(p_{h}^{1}(y), \ldots, p_{h}^{\mathcal{N}}(y)\right)^{\top}$. The high-fidelity (Petrov)-Galerkin approximation given any $y \in U$, find $p_{h}(y) \in \mathcal{X}_{h}$ such that $A\left(p_{h}(y), v_{h} ; y\right)=F\left(v_{h}\right) \quad \forall v_{h} \in \mathcal{Y}_{h}$.

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given any $y \in U$, find $\mathbf{p}_{h}(y) \in \mathbb{R}^{\mathcal{N}}$ such that $\left(\mathbb{A}_{h}^{0}+\sum_{j \in \mathbb{J}} y_{j} \mathbb{A}_{h}^{j}\right) \mathbf{p}_{h}(y)=\mathbf{f}_{h}$,
which is a $\mathcal{N} \times \mathcal{N}$ system, requiring large-scale computation when $\mathcal{N}$ is very large.

## Reduced basis approximation: low-dimensional manifold

Reducibility: the solution manifold $\mathcal{M}=\left\{p_{h}(y) \in \mathcal{X}_{h}, y \in U\right\}$ is low-dimensional.


## Mathematically, the best approximation error decays very fast

Kolmogorov $N$-width: $d_{N}\left(\mathcal{X}_{h}, \mathcal{M}\right):=\inf \operatorname{sun} \inf \|v-w\|_{\nu} \equiv \inf \operatorname{dist}\left(\mathcal{Z}_{N}, \mathcal{M}\right)$

Look for a low-dimensional reduced basis space $\mathcal{X}_{N} \subset \mathcal{M}$ such that
reduced hasis error: $\sigma_{N}\left(\mathcal{X}_{N}, \mathcal{M}\right):=\operatorname{sun} \inf \| v_{v}-w_{N}=\operatorname{dist}\left(\mathcal{X}_{N}, \mathcal{M}\right)$

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$$

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: $\mathcal{X}_{N} \subset \mathcal{X}_{h}$ and $\mathcal{Y}_{N} \subset \mathcal{Y}_{h}$;
- Let $\left(w_{N}^{n}\right)_{n=1}^{N}$ and $\left(v_{N}^{n}\right)_{n=1}^{N}$ denote the bases of $\mathcal{X}_{N}$ and $\mathcal{Y}_{N}$;



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\begin{equation*}
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\end{equation*}
$$

with $\mathbf{p}_{N}(y)=\left(p_{N}^{1}(y), \ldots, p_{N}^{N}(y)\right)^{\top}$. The reduced basis (Petrov)-Galerkin approximation given any $y \in U$, find $p_{N}(y) \in \mathcal{X}_{N}$ such that $A\left(p_{N}(y), v_{N} ; y\right)=F\left(v_{N}\right) \quad \forall v_{N} \in \mathcal{Y}_{N}$.


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with $\mathbf{p}_{N}(y)=\left(p_{N}^{1}(y), \ldots, p_{N}^{N}(y)\right)^{\top}$. The reduced basis (Petrov)-Galerkin approximation

$$
\begin{equation*}
\text { given any } y \in U \text {, find } p_{N}(y) \in \mathcal{X}_{N} \text { such that } A\left(p_{N}(y), v_{N} ; y\right)=F\left(v_{N}\right) \quad \forall v_{N} \in \mathcal{Y}_{N} . \tag{15}
\end{equation*}
$$

Let $\mathbb{W}=\left(\mathbf{w}_{N}^{1}, \ldots, \mathbf{w}_{N}^{N}\right)$ and $\mathbb{V}=\left(\mathbf{v}_{N}^{1}, \ldots, \mathbf{v}_{N}^{N}\right), \mathbb{A}_{N}^{j}=\mathbb{V}^{\top} \mathbb{A}_{h}^{j} \mathbb{W}, j \in\{0\} \cup \mathbb{I} ; \mathbf{f}_{N}=\mathbb{V}^{\top} \mathbf{f}_{h}$.
given any $y \in U$, find $\mathbf{p}_{N}(y) \in \mathbb{R}^{N}$ such that $\left(\mathbb{A}_{N}^{0}+\sum_{j \in \mathbb{J}} y_{j} \mathbb{A}_{N}^{j}\right) \mathbf{p}_{N}(y)=\mathbf{f}_{N}$.
which is a $N \times N$ system, needs small-scale computation as $N \ll \mathcal{N}$, e.g. $(10 \sim 100)$.

## Reduced basis approximation: construction of reduced spaces

## Greedy algorithm [Patera and Rozza, 2007]

Initialize $\mathcal{X}_{1}=\operatorname{span}\left\{p_{h}\left(y^{(1)}\right)\right\}$ at some random sample $y^{(1)}$, then for $N=2,3, \ldots$,

$$
\begin{equation*}
y^{(N)}=\underset{y \in U}{\operatorname{argsup}}\left\|p_{h}(y)-p_{N-1}(y)\right\| \mathcal{X} \quad \text { or } \quad y^{(N)}=\underset{y \in U}{\operatorname{argsup}}\left|\Theta_{h}(y)-\Theta_{N-1}(y)\right| \tag{17}
\end{equation*}
$$

and the reduced space $\mathcal{X}_{N}$ can be constructed by the snapshots

$$
\begin{equation*}
\mathcal{X}_{N}=\mathcal{X}_{N-1} \oplus \operatorname{span}\left\{p_{h}\left(y^{(N)}\right)\right\} . \tag{18}
\end{equation*}
$$

Gram-Schmidt process $\rightarrow$ orthnormal bases $\left(w_{N}^{n}\right)_{n=1}^{N}$ 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 $v_{N}^{n}(y) \in \mathcal{V}_{h}$ such that $\left(v_{N}^{n}(y), v_{h}\right) \nu_{h}=A\left(w_{N}^{n}, v_{h} ; y\right)$
Let $\mathbb{A}_{N}^{j, j}=\left(\mathbb{A}_{h}^{j} \mathbb{W}\right)^{\top} \mathbb{M}_{h}^{-1} \mathbb{A}_{h}^{j} \mathbb{W}$, and $\mathbb{I}_{N}^{j}=\left(\mathbb{A}_{h}^{j} \mathbb{W}\right)^{\top} \mathbb{M}_{h}^{-1} \mathbf{f}_{h} ;$ we solve the $N \times N$ system



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$$
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## Reduced basis approximation: construction of reduced spaces

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$$

$$
\text { Let } \mathbb{A}_{N}^{j, j^{\prime}}=\left(\mathbb{A}_{h}^{j} \mathbb{W}\right)^{\top} \mathbb{M}_{h}^{-1} \mathbb{A}_{h}^{j^{\prime} \mathbb{W}} \text {, and } \mathbf{f}_{N}^{j}=\left(\mathbb{A}_{h}^{j} \mathbb{W}\right)^{\top} \mathbb{M}_{h}^{-1} \mathbf{f}_{h} ; \text { we solve the } N \times N \text { system }
$$

$$
\begin{equation*}
\left(\mathbb{A}_{N}^{0,0}+2 \sum_{j \in \mathbb{J}} y_{j} \mathbb{A}_{N}^{0, j}+\sum_{j \in \mathbb{J}} \sum_{j^{\prime} \in \mathbb{J}} y_{j} y_{j^{\prime}} \mathbb{A}_{N}^{j, j^{\prime}}\right) \mathbf{p}_{N}(y)=\mathbf{f}_{N}^{0}+\sum_{j \in \mathbb{J}} y_{j} \mathbf{f}_{N}^{j} . \tag{20}
\end{equation*}
$$

## Reduced basis approximation: a posteriori error estimators I

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

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

which can be expanded as

$$
\begin{equation*}
\Theta_{h}(y)=\Theta_{N}(y)+\left.\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(p_{h}(y)-p_{N}(y)\right)+O\left(| | p_{h}(y)-p_{N}(y) \|_{\mathcal{X}}^{2}\right) . \tag{21}
\end{equation*}
$$

We can estimate the error by
$\left|\Theta_{h}(y)-\Theta_{N}(y)\right| \approx\left|\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(p_{h}(y)-p_{N}(y)\right)\left|\leq\left|\left|\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\right|\right|_{\mathcal{X}^{\prime}}| | p_{h}(y)-p_{N}(y) \|_{\mathcal{X}}=: \Delta_{N}^{(1)}(y)$.
Here, the reduced solution error can be bounded by
where the residual $R_{h}(\cdot ; y) \in \mathcal{Y}^{\prime}$, defined as
and the inf-sup constant $\beta_{h}(y)$ is uniformly bounded from below by $\beta_{h}^{L B}$

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$$

Here, the reduced solution error can be bounded by

$$
\left\|p_{h}(y)-p_{N}(y)\right\|_{\mathcal{X}} \leq \frac{\left\|R_{h}(\cdot ; y)\right\|_{\mathcal{Y}^{\prime}}}{\beta_{h}(y)}=: \triangle_{N}^{p}(y),
$$

where the residual $R_{h}(\cdot ; y) \in \mathcal{Y}^{\prime}$, defined as

$$
R_{h}\left(v_{h} ; y\right)=F\left(v_{h}\right)-A\left(p_{N}(y), v_{h} ; y\right) \quad \forall v_{h} \in \mathcal{Y}_{h},
$$

and the inf-sup constant $\beta_{h}(y)$ is uniformly bounded from below by $\beta_{h}^{L B}$.

## 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 $A\left(w_{h}, \psi_{h} ; y\right)=\left.\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(w_{h}\right) \quad \forall w_{h} \in \mathcal{X}_{h}$.

We may approximate this high-fidelity solution with a reduced dual solution by solving
find $\psi_{N_{d u}}(y) \in \mathcal{Y}_{N_{d u}}$ such that $A\left(w_{N_{d u}}^{d u}, \psi_{N_{d u}} ; y\right)=\left.\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(w_{N_{d u}}^{d u}\right) \quad \forall w_{N_{d u}}^{d u} \in \mathcal{X}_{N_{d u}}$.
The second error estimator (dual-weighted residual) is simply defined as

A closer look at the residual (by Galerkin orthogonality)

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

## 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 $A\left(w_{h}, \psi_{h} ; y\right)=\left.\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(w_{h}\right) \quad \forall w_{h} \in \mathcal{X}_{h}$.
We may approximate this high-fidelity solution with a reduced dual solution by solving

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\end{equation*}
$$

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

$$
\begin{equation*}
\triangle_{N}^{(2)}(y):=R\left(\psi_{N_{d u}}(y) ; y\right)=\mathbf{f}_{h}^{\top} \mathbb{W}_{d u} \psi_{N_{d u}}(y)-\sum_{j \in\{0\} \cup J} y_{j}\left(\mathbf{p}_{N}(y)\right)^{\top} \mathbb{W}^{\top} \mathbb{A}_{h}^{j} \mathbb{W}_{d u} \psi_{N_{d u}}(y) \tag{23}
\end{equation*}
$$

A closer look at the residual (by Galerkin orthogonality):

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## 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 $A\left(w_{h}, \psi_{h} ; y\right)=\left.\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(w_{h}\right) \quad \forall w_{h} \in \mathcal{X}_{h}$.

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\end{equation*}
$$

A closer look at the residual (by Galerkin orthogonality):

$$
\begin{equation*}
R\left(\psi_{h}(y) ; y\right)=A\left(p_{h}(y)-p_{N}(y), \psi_{h}(y) ; y\right)=\left.\frac{\partial \Theta_{h}}{\partial p_{h}}\right|_{p_{N}(y)}\left(p_{h}(y)-p_{N}(y)\right), \tag{24}
\end{equation*}
$$

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

$$
\begin{equation*}
R\left(\psi_{h}(y) ; y\right)-\triangle_{N}^{(2)}(y)=R\left(e_{h}^{d u}(y) ; y\right)=A\left(e_{h}(y), e_{h}^{d u}(y) ; y\right) \leq \gamma_{h}(y)\left\|e_{h}(y)\right\| \mathcal{X}\left\|e_{h}^{d u}(y)\right\| \mathcal{V} \tag{25}
\end{equation*}
$$

where we denote the reduced errors $e_{h}(y)=p_{h}(y)-p_{N}(y)$ and $e_{h}^{d u}(y)=\psi_{h}(y)-\psi_{N_{d t}}(y)$.

## Reduced basis approximation: a posteriori error estimators III

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

$$
\begin{equation*}
\Theta_{N}^{c}(y)=\Theta_{N}(y)+\triangle_{N}^{(2)}(y) \tag{26}
\end{equation*}
$$

The last term in the expansion can be further expanded as


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

$\square$
Note that

The second (dual-weighted residual) error estimator is the cheapest to evaluate.

## Reduced basis approximation: a posteriori error estimators III

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

$$
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The last term in the expansion can be further expanded as
$O\left(\left\|p_{h}(y)-p_{N}(y)\right\|_{\mathcal{X}}^{2}\right)=\left.\frac{1}{2} \frac{\partial^{2} \Theta_{h}}{\partial p_{h}^{2}}\right|_{p_{N}(y)}\left(p_{h}(y)-p_{N}(y), p_{h}(y)-p_{N}(y)\right)+O\left(\left\|p_{h}(y)-p_{N}(y)\right\|_{\mathcal{X}}^{3}\right)$.
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where (note $\left|\Theta_{h}(y)-\Theta_{N}^{c}(y)\right| \approx$ ( first term $\left.-\triangle_{N}^{(2)}\right)+$ second term )
$\qquad$

## Reduced basis approximation: a posteriori error estimators III

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

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\Theta_{N}^{c}(y)=\Theta_{N}(y)+\triangle_{N}^{(2)}(y) \tag{26}
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\begin{equation*}
\triangle_{N}^{(3)}(y):=\max \left\{\triangle_{N}^{(4)}(y), \triangle_{N}^{(5)}(y)\right\} \tag{27}
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Note that $\triangle_{N}^{(4)}$ and $\triangle_{N}^{(5)}$ exhibit a quadratic dependence on the reduced solution error.
The second (dual-weighted residual) error estimator is the cheapest to evaluate.

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## Reduced basis approximation: an adaptive greedy algorithm

Adaptively construct the reduced bases using sparse grid nodes as training samples.

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

Initialization: specify tolerance $\epsilon_{t}$, set $N=1$, solve the hiah-fide lity problem at $y_{1}^{1}$, the root node in the sparse grid, and construct the first reduced space $\mathcal{X}_{1}=\operatorname{span}\left\{p_{h}\left(y_{1}^{1}\right)\right\}$ While sparse grid construction continues
at each new index $\boldsymbol{i}$, update the training set $\Xi_{\text {train }}=\Xi_{\triangle}^{i}$;
While max
end

Replace high-fidelity solve by reduced basis solve at almost all sparse grid nodes.

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at each new index $i$, update the training set $\Xi_{\text {train }}=\Xi_{\triangle}^{i}$;
set $y^{(N+1)}=\operatorname{argmax}_{y \in \Xi_{\min }} \triangle_{N}(y)$
solve high-fidelity problem at $y^{(N+1)}$ to obtain $p_{n}(y)$
update $X_{N+1}=X_{N} \in \operatorname{span}\left\{p_{n}(y\right.$
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$$
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$$

solve high-fidelity problem at $y^{(N+1)}$ to obtain $p_{h}\left(y^{(N+1)}\right)$;
update $\mathcal{X}_{N+1}=\mathcal{X}_{N} \oplus \operatorname{span}\left\{p_{h}\left(y^{(N+1)}\right)\right\}$;
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Replace high-fidelity solve by reduced basis solve at almost all sparse grid nodes.

## A priori error estimates

## Assumption [Schwab and Stuart, 2012]

There exist $0<a_{\text {min }} \leq a_{\text {max }}<\infty$, such that $\forall z \in \mathcal{U}:=\bigotimes_{j \in J}\left\{z \in \mathbb{C}^{J}:\left|z_{j}\right| \leq 1\right\}$

$$
\begin{equation*}
a_{\text {min }} \leq \Re(u(x, z)) \leq|u(x, z)| \leq a_{\max }, \quad \forall x \in D \tag{29}
\end{equation*}
$$

There exists a constant $0<\alpha<1$, such that (recall $u(y)=\psi_{0}+\sum_{j \in \mathrm{~J}} y_{j} \psi_{j}$ )

$$
\begin{equation*}
\sum_{j \in J}\left\|\psi_{j}\right\|_{L^{\infty}(D)}^{\alpha}<\infty . \tag{30}
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## Global approximation

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


quadrature error

high-fidelity error

reduced basis error

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

and

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

## A priori error estimates

## Sparse grid approximation error [Schillings and Schwab, 2013]

$$
\left|\Theta(y)-\Theta_{s}(y)\right| \leq C M^{-s} \text { and }\left|Z-Z_{s}\right| \leq C M^{-s}, \quad s=\frac{1}{\alpha}-1 .
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## High-fidelity approximation error

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

## Global approximation error

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Global approximation error

$$
\begin{gathered}
\left|\Theta(y)-\Theta_{s, h, r}(y)\right| \leq C_{0} M^{-s}+C_{1} h^{t}+C_{2} N^{-s} . \\
\left|Z-Z_{s, h, r}\right| \leq C_{0} M^{-s}+C_{1} h^{t}+C_{2} N^{-s} .
\end{gathered}
$$

## 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 $\psi_{j}=0.95 j^{-2} \chi_{D_{j}}, j \in \mathbb{J}$, 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).

## Numerical experiments: high-fidelity approximation error



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

$$
\text { effectivity }=\frac{\triangle_{N}}{\left|\Theta_{h}(y)-\Theta_{N}(y)\right|}
$$





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

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Figure: Left: effect of correction $E_{2} / E_{1}$ with $E_{2}=\left|\Theta_{h}(y)-\Theta_{N}^{c}(y)\right|$ and $E_{1}=\left|\Theta_{h}(y)-\Theta_{N}(y)\right|$; 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

$$
\max _{y \in \Xi_{\text {test }}} \frac{\left|\Theta_{h}(y)-\Theta_{N}(y)\right|}{\Theta_{h}(y)}
$$




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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## Conclusion and perspective

## 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 problerns.
- 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.
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## References I

(Rinev, P., Cohen, A., Dahmen, W., DeVore, R., Petrova, G., and Wojtaszczyk, P. (2011).

Convergence rates for greedy algorithms in reduced basis methods.
SIAM Journal of Mathematical Analysis, 43(3):1457-1472.
Chen, P. and Quarteroni, A. (2014).
A new algorithm for high-dimensional uncertainty problems based on dimension-adaptive and reduced basis methods.
EPFL, MATHICSE Report 09, submitted.
Cohen, A. and DeVore, R. (2014).
Kolmogorov widths under holomorphic mappings.

- Gerstner, T. and Griebel, M. (2003).

Dimension-adaptive tensor-product quadrature.
Computing, 71(1):65-87.
Patera, A. and Rozza, G. (2007).
Reduced basis approximation and a posteriori error estimation for parametrized partial differential equations.
Copyright MIT, http://augustine.mit.edu.

## References II

Schillings, C. and Schwab, C. (2013).
Sparse, adaptive smolyak quadratures for bayesian inverse problems.
Inverse Problems, 29(6).
Schwab, C. and Stuart, A. (2012).
Sparse deterministic approximation of bayesian inverse problems.
Inverse Problems, 28(4):045003.
圊 Smolyak, S. (1963).
Quadrature and interpolation formulas for tensor products of certain classes of functions.
In Doklady Akademii Nauk SSSR, volume 4, pages 240-243.
Stuart, A. (2010).
Inverse problems: a Bayesian perspective.
Acta Numerica, 19(1):451-559.

## Thank you for your attention!

