The Reduced-Basis (RB) method for Uncertainty Quantification (UQ)

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ICMS, Edinburgh May 2010

Outline

UQ: BVP with random parameter

uncertainty propagation – (Bayesian) parameter estimation

For PDEs with stochastic coefficients, e.g. diffusion $\boldsymbol{A}$

$$-\operatorname{div}(\boldsymbol{A}\nabla u) = f \qquad (1)$$

how to compute expensive (high-dim.) solutions to (1) ?

1. Sample u (+ outputs: moments...) by Monte-Carlo (MC)
2. Accelerates the "many-query" problem by RB method

Notice that:

- RB method can also reduce other discretizations (e.g. quad. formula invoking indep. parametrized problems)
- naive MC is often less favourable than deterministic quad. (in small dim.), but OK with efficient variance reduction

Outline

Problem: compute many expensive input-output relationships

For many *input* parameters μ, compute an expensive $u(\mu) \in X$.

RB = project $u(\mu)$ on best linear space spanned by "snapshots"

1. identify "offline": $X_N = \mathrm{Span}\left(u(\mu_n^N), n = 1, \ldots, N\right)$
2. compute fast at any μ: $u_N(\mu) \in \operatorname*{arginf}_{v \in X_N} \|u(\mu) - v\|_{\mu,X}$

Remarks:

- "Online" computations can be certified $\sup_{\mu} \|u(\mu) - u_N(\mu)\|_{\mu,X} \leq \varepsilon$
- RB (Patera-Maday®) ought to be a good strategy if…
  - $\bigcup_{\mu} \{u(\mu)\}$ is close to a small-dimensional vector space
  - (offline+online) effort = less expensive at fixed accuracy ε

Example: μ-elliptic variational pb. $a(u(\mu), v; \mu) = l(v)\,, \ \forall v \in X$

Given μ, find $u(\mu) \in X$ solution to $-\operatorname{div}(\boldsymbol{A}(\mu)\nabla u(\mu)) = f + \text{ BC}$

u_N best approx. in energy (Galerkin): $\|\cdot\|_{\mu,X} = \sqrt{a(\cdot,\cdot;\mu)}$

X_N N-linear space minimizing L^∞-width: $\sup_\mu \|u(\mu) - u_N(\mu)\|_{\mu,X}$

- goal-oriented cases (like *homogenization*) $\rightarrow$ RB also for adjoint eq.

This is a "best N-linear space" approximation problem:

computing minimizers of $\inf_{\mu_1,\dots,\mu_N} \left(\sup_\mu \|u(\mu) - u_N(\mu)\|_{\mu,X} \right)$ hard !

Practical approach

Assume a good discretization $X_{\mathcal{N}}$ of X (d.o.f. $\mathcal{N} \gg 1$)

1. *a posteriori* estimators $\Delta_{\mathcal{N},N}(\mu) \geq \|u_{\mathcal{N}}(\mu) - u_N(\mu)\|_{\mu,X}$,
2. Greedy algorithms selecting *iteratively* $(n = 1, \dots)$ $\mu_n^N = \mu_n$ within a training sample of μ while $\sup_{\mu \in \text{sample}} \Delta_{\mathcal{N},N}(\mu) \leq \varepsilon$

$$\mu_1 = rand(); \; \mu_{n+1} \in \left(\sup_{\mu \in \text{sample}} \Delta_{\mathcal{N},n}(\mu) \right), \; n = 1, \dots, N-1$$

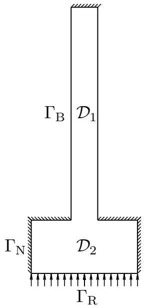
Outline

A simple uncertainty propagation problem

$$-\mathrm{div}\,(\boldsymbol{A}(x)\nabla u(x,\omega)) = 0 \text{ in } \mathcal{D} \qquad (2)$$

$$\boldsymbol{n}(x)^T \boldsymbol{A}(x)\nabla u(x,\omega) + B(x,\omega)\, u(x,\omega) = g(x) \text{ on } \partial\mathcal{D} \qquad (3)$$

$$B = B1_{\Gamma_B} > 0 \quad g = g1_{\Gamma_R} \in L^2(\partial\mathcal{D}) \qquad s(\omega) = \int_{\Gamma_R} g u(\cdot,\omega)$$



$$\boldsymbol{A}(x) = \begin{pmatrix} k(x) & 0 \\ 0 & k(x) \end{pmatrix}$$

$$k = \begin{cases} k_1 \text{ in } \mathcal{D}_1 \\ k_2 \text{ in } \mathcal{D}_2 \end{cases}$$

$$\partial\mathcal{D} = \Gamma_R \cup \Gamma_N \cup \Gamma_B$$

$$(\Gamma_R \cap \Gamma_N \cap \Gamma_B = \emptyset)$$

RB technicalities

parametrically-affine formulation

- Sample output distribution: MC with $B^m(\cdot,\omega), m = 1 \dots M$
- Given $B^m(\cdot,\omega)$, accurate approx.: Finite-Element $u_\mathcal{N} \in X_\mathcal{N}$

$$a(u_\mathcal{N}, v_\mathcal{N}; \underbrace{k_1, k_2, B(\cdot,\omega)}_{\mu}) = l(v_\mathcal{N}; g) \quad \forall v_\mathcal{N} \in X_\mathcal{N} \subset X := H^1(\mathcal{D})$$

Issue: many realizations ($\mathcal{N} \gg 1$ d.o.f.) $\rightarrow$ **RB**(μ)

- Efficient reduction with RB to $X_N \subset X_\mathcal{N}$ needs
  - a fast projector in X_N (Galerkin)
  - a fast a posteriori error estimator for $\|u_\mathcal{N} - u_N\|_X$

$B(\cdot,\omega)$ = infinitely many coefficients ! $\Rightarrow$ e.g. parametrically-affine decomposition with Karhunen–Loève

Karhunen–Loève expansion of random input

$$B(x,\omega) = \bar{B}\left(G(x) + \Upsilon \sum_{k=1}^{\mathcal{K}} \sqrt{\lambda_k}\Phi_k(x)Z_k(\omega)\right)$$

- $\bar{B}, \Upsilon$ = positive amplitude parameters ($\int_{\partial\mathcal{D}} G = 1$)
- $\mathcal{K}$ = rank (possibly ∞) of covariance operator for $B(x,\omega)\ldots$
- $\ldots$with eigenpairs $\left(\bar{B}\Upsilon^2\lambda_k, \Phi_k(x)\right)_k$ ($\int_{\partial\mathcal{D}} \mathrm{Var}(B) = \bar{B}\Upsilon^2$)
- $(Z_k(\omega))_{1\le k\le\mathcal{K}}$ = $L^2_P(\Omega)$-orthonormal random variables

$$\Rightarrow a(u,v;\mu) \equiv k_1 a_1(u,v) + k_2 a_2(u,v) + \sum_k \underbrace{\left(\sqrt{\lambda_k}Z_k(\omega)\right)}_{\mu_k(\omega)} b_k(u,v)$$

Mathematical technicalities

some limitations (at least for simple, rigorous error estimators)

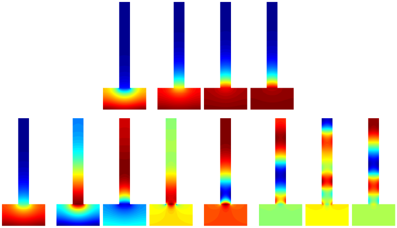
- RB method applies to <u>truncated problems</u>
  with KL at finite order $K \leq \mathcal{K} \rightarrow \Delta_{N,K}((\mu_k)_{k\leq K})$
- Only for random fields $B \in L^\infty$
  ($\Rightarrow$ well-posedness + existence of KL expansion)
  with uniformly converging KL expansions
  ($\Leftarrow |Z_k|, \|\Phi_k\|$ uniformly bounded, $\sum \sqrt{\lambda_k} < \infty$)
- Only when B and KL expansions $B_K > B_-$ uniformly
  ($\Leftarrow \Upsilon \leq \Upsilon_{\max}$)

Example of reduced basis

H^1 orthonormalized for well-conditioned reduced problems

Greedy algorithm : solutions generated by gaussian covariance kernels $\exp(-|x-y|^2/\delta^2)$

$k_1 = 1$, $k_2 \in (.1, 10)$, $\bar{B} = (.1, 1)$, $G(x) \equiv 1$, $\delta = .5$, $\mathcal{K} = 25$, $\Upsilon = .058$, $Z_k \sim \mathcal{U}(-1, 1)$, $\forall k \leq K = 25$



[3] S. B. C. Le Bris Y. Maday N.C. Nguyen A.T. Patera, A Reduced Basis Approach for Variational Problems with Stochastic Parameters: Application to Heat Conduction with Variable Robin Coefficient,CMAME 198,2009.

Output: response surfaces

sample $(Z_k^m)_{k\leq K} \to u_{N,K}^m \to s_{N,K}^m \to E_M[s_{N,K}] = \frac{1}{M}\sum_{m=1}^M s_{N,K}^m$

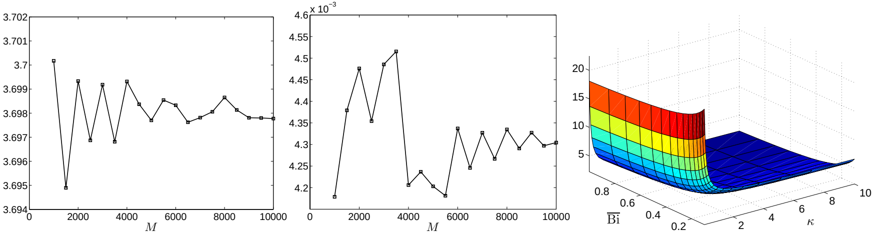


Figure: Mean $E_M[s_{N,K}]$ and variance $V_M[s_{N,K}]$ w.r.t. M at $k_2 = 2.0$, $\bar{B} = 0.5$ and variations of mean with $(k_2, \bar{B})$.

Error bounds (global = truncation + reduction)

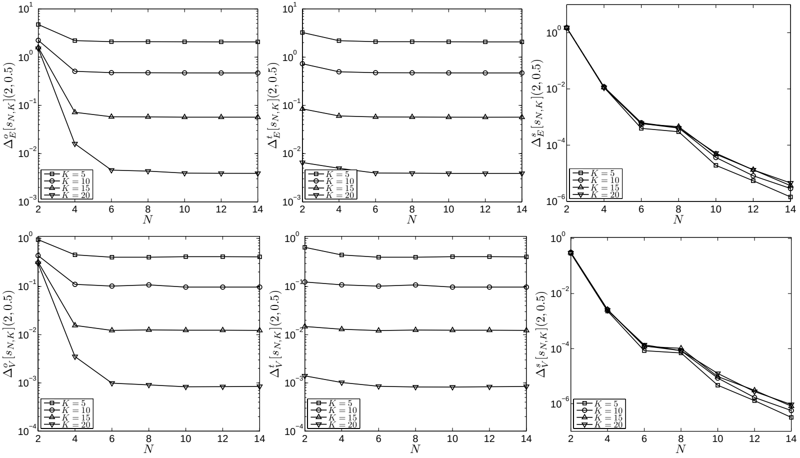


Figure: Error bounds for (a) $E(S)$ and (b) $V(S)$ w.r.t. N, K.

Outline

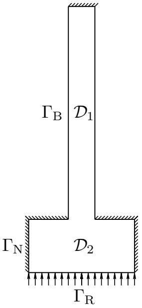
Classical RB in parameter estimation

One approach to parameter estimation with Bayesian inferences

$$-\mathrm{div}\,(\boldsymbol{A}(x)\nabla u(x,\omega)) = 0 \text{ in } \mathcal{D} \tag{4}$$

$$\boldsymbol{n}(x)^{\mathrm{T}}\,\boldsymbol{A}(x)\nabla u(x,\omega) + B\,u(x,\omega) = g(x) \text{ on } \partial\mathcal{D} \tag{5}$$

$$B = B1_{\Gamma_{\mathrm{B}}} > 0 \quad g = g1_{\Gamma_{\mathrm{R}}} \in L^2(\partial\mathcal{D}) \qquad s(\omega) = \int_{\Gamma_{\mathrm{R}}} gu(\cdot,\omega)$$



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$$\partial\mathcal{D} = \Gamma_R \cup \Gamma_N \cup \Gamma_B$$

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Parameter estimation from Bayesian inference

The MMSE case

Standard RB useful to MMSE e.g.
(exactly like for statistics of uncertainty propagation in PDEs !)

$$\hat{k}_2(s^\star) = E(k_2|s+\xi=s^\star) = \int k_2 \pi(k_2|s(u(\underbrace{k_2}_{\mu})) + \xi = s^\star) dk_2$$

where observations $s+\xi = I^\star$ are spoiled by $\xi \sim f$
and a prior $k_2 \sim \pi$ gives a Bayes formula

$$\pi(k_2|s+\xi=s^\star) = \frac{f(s^\star - s|k_2)\pi(k_2)}{P(s+\xi=s^\star)}$$

RB $\rightarrow$ OK with deterministic quadrature for MMSE.
See [4] (parametrized parabolic PDEs).

Nguyen, N.C., Rozza, G., Huynh, D.B.P., Patera, A.T. Reduced basis approximation and a posteriori error estimation for parametrized parabolic pdes; application to real-time bayesian parameter estimation. Computational Methods for Large Scale Inverse Problems and Uncertainty Quantification, John Wiley & Sons, UK (2009).

On-going with Monte-Carlo (higher dimensions)

Outline

MC acceleration

reduce statistical error

Response surfaces, parameter estimation: many MC samples
$\longrightarrow$ opportunity for RB ideas in variance reduction too !

First applied to parametrized SDEs (rheology, finance) [2]

S. B., T. Lelièvre A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm CMS 8 spec. iss. (P. Zhang ed.), 2010 (arXiv:0906.3600).

Outline

Computational reductions and RB ideas

A general philosophy able to adapt

- UQ: many reduction opportunities
- *Efficient certified reduction* possible with the (now standard) RB method [Patera-Maday®]
- Combination with fast MC approach possible with control-variates (on-going)

For Further Reading I

S.B., C. Le Bris, T. Lelièvre, Y. Maday, N.C. Nguyen and A.T. Patera
Reduced basis techniques for stochastic problems
ArCME special issue (E. Cueto, F. Chinesta, P. Ladeveze and A. Nouy ed.), 2010 (arXiv:1004.0357).

S. B., T. Lelièvre
A variance reduction method for parametrized stochastic differential equations using the reduced basis paradigm
CMS 8 spec. iss. (P. Zhang ed.), 2010 (arXiv:0906.3600).

For Further Reading II

- S. B., C. Le Bris, Y. Maday, N.C. Nguyen and A.T. Patera
  A Reduced Basis Approach for Variational Problems with Stochastic Parameters: Application to Heat Conduction with Variable Robin Coefficient
  CMAME 198(41–44):3187–3206, 2009.
- N.C.Nguyen, G. Rozza, D.B.P. Huynh, A.T. Patera
  Reduced basis approximation and a posteriori error estimation for parametrized parabolic pdes; application to real-time bayesian parameter estimation.
  Computational Methods for Large Scale Inverse Problems and Uncertainty Quantification, John Wiley & Sons, UK (2009)

Outline

Parametrized r.v. $Z^\mu \in L^2(\Omega)$ in Monte-Carlo

Goal: compute expectation $E(Z^\mu)$ for many μ.

Monte-Carlo with confidence intervals (CLT+Slutsky) $\forall a > 0$

$$\mathrm{E}_M(Z^\mu) := \frac{1}{M}\sum_{m=1}^{M} Z_m^\mu \xrightarrow[M\to\infty]{P-a.s.} E(Z^\mu) \qquad \mathrm{Var}_M(Z^\mu) = \dots$$

$$P\left(|\mathrm{E}_M(Z^\mu) - E(Z^\mu)| \le a\sqrt{\frac{\mathrm{Var}_M(Z^\mu)}{M}}\right) \xrightarrow[M\to\infty]{} \int_{-a}^{a} \frac{e^{-x^2/2}}{\sqrt{2\pi}} dx$$

Faster MC with variance reduced by control variates Y^μ:

Compute $E(Z^\mu) = E(Z^\mu - Y^\mu) + E(Y^\mu)$ where

- $E(Y^\mu)$ is known (here $E(Y^\mu) = 0$)
- $Var(Z^\mu) \ge Var(Z^\mu - Y^\mu)$.

Control variates: practical variance reduction

Ideally $Y^\mu = Z^\mu - E(Z^\mu) \Rightarrow Var(Z^\mu - Y^\mu) = 0$, but in practice:

Compute $\tilde{Y}^\mu \approx Y^\mu$ minimizing

$$Var(Z^\mu - \tilde{Y}^\mu) = E\left(\left|(Z^\mu - E(Z^\mu)) - \tilde{Y}^\mu\right|^2\right) = E\left(\left|Y^\mu - \tilde{Y}^\mu\right|^2\right)$$

Faster MC with RB approach :

$$\tilde{Y}^\mu := \sum_{n=1}^{N} \alpha_n(\mu) Y^{\mu_n} = \sum_{n=1}^{N} \alpha_n(\mu) \left(Z^{\mu_n} - E(Z^{\mu_n})\right)$$

where the $\alpha_n(\mu)$ minimize $Var(Z^\mu - \tilde{Y}^\mu)$

$$\mathrm{E}_{\mathrm{M_{small}}}\left(Z^\mu - \tilde{Y}^\mu\right) = \frac{1}{\mathrm{M_{small}}} \sum_{m=1}^{\mathrm{M_{small}}} (Z^\mu_m - \tilde{Y}^\mu_m) \xrightarrow[\mathrm{M_{small}} \to \infty]{P-a.s.} E(Z^\mu).$$

Control variates: practical variance reduction

Ideally $Y^\mu = Z^\mu - E(Z^\mu) \Rightarrow Var(Z^\mu - Y^\mu) = 0$, but in practice:

Compute $\tilde{Y}^\mu \approx Y^\mu$ minimizing

$$Var(Z^\mu - \tilde{Y}^\mu) = E\left(\left|(Z^\mu - E(Z^\mu)) - \tilde{Y}^\mu\right|^2\right) = E\left(\left|Y^\mu - \tilde{Y}^\mu\right|^2\right)$$

Faster MC with RB approach :

$$\tilde{Y}^\mu := \sum_{n=1}^{N} \alpha_n(\mu) Y^{\mu_n} \approx \sum_{n=1}^{N} \alpha_n(\mu) \left(Z^{\mu_n} - \mathrm{E}_{\mathrm{M}_{\mathrm{large}}}(Z^{\mu_n})\right)$$

where the $\alpha_n(\mu)$ minimize $\mathrm{Var}_{\mathrm{M}_{\mathrm{small}}}(Z^\mu - \tilde{Y}^\mu)$

$$\mathrm{E}_{\mathrm{M}_{\mathrm{small}}}\left(Z^\mu - \tilde{Y}^\mu\right) = \frac{1}{\mathrm{M}_{\mathrm{small}}} \sum_{m=1}^{\mathrm{M}_{\mathrm{small}}} (Z^\mu_m - \tilde{Y}^\mu_m) \xrightarrow[\mathrm{M}_{\mathrm{small}} \to \infty]{P-a.s.} E(Z^\mu).$$

Effective RB control variates method in practice

Effective numerical variance minimizations:

For all μ, solve the least-square problem by usual methods

$$\inf_{\{\alpha_1(\mu),\dots,\alpha_N(\mu)\}} \mathrm{Var}_{\mathrm{M_{small}}}\left(Z^\mu - \sum_{n=1}^{N} \alpha_n(\mu) \left(Z^{\mu_n} - E(Z^{\mu_n}) \right) \right)$$

For instance, SVD or QR for the normal equations ($i = 1, \dots, N$)
$\sum_{j=1}^N \mathrm{Cov}_{\mathrm{M_{small}}}\left(Z^{\mu_i}, Z^{\mu_j}\right) \alpha_j^\mu = \mathrm{Cov}_{\mathrm{M_{small}}}\left(Z^{\mu_i}, Z^\mu\right)$

Computational gains:

Only in the many-query limit = many μ !
(Offline: N expensive computations $\mathrm{E}_{\mathrm{M_{large}}}(Z^{\mu_n})$ + greedy)
$\Rightarrow$ OK for many observations $s^\star$, or a large response surface !