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Goal-oriented error estimation for reduced basis method, with application to certified sensitivity analysis

Alexandre Janon , Maëlle Nodet , and Clémentine Prieur *

Abstract. The reduced basis method is a powerful model reduction technique designed to speed up the computation of multiple numerical solutions of parameterized partial differential equations (PDEs). We consider a quantity of interest, which is a linear functional of the parameterized PDE solution. Compared to the original quantity of interest, the quantity of interest computed using the reduced model is tainted by a reduction error. We present a new, efficiently and explicitly computable bound for this error, and we show on different examples that this error bound is more precise than existing ones. We also present an application of our work to certified sensitivity analysis studies.

Key words. reduced basis method, surrogate model, reduced order modelling, response surface method, scientific computation, sensitivity analysis, Sobol index computation, Monte-Carlo method

AMS subject classifications. 65M15

Introduction. A large number of mathematical models are based on partial differential equations (PDEs). These models require input data (e.g., the physical features of the considered system, the geometry of the domain, the external forces...) which enter in the PDE as *parameters*. In many applications (for instance, design optimization, data assimilation, or uncertainty quantification), one has to numerically compute the solution of a parametrized partial differential equation for a large number of values of the parameters. In such a case, it is generally interesting, in terms of computation time, to perform all possible parameter-independent computations in an *offline* phase, which is done only once, and to call an *online* phase for each required value of the parameter, during which the information gathered in the offline phase can be used to speed-up the computation of an approximate solution of the PDE, and, hence, to reduce the marginal (ie., per parameter) computation cost.

The reduced basis method ([7]) is a way of specifying such offline and online phases, which has been successfully applied to various well-known PDEs ([3, 6, 15]). One should note that, in the reduced basis (RB) method, the online phase does not compute a solution which is strictly identical to the numerical PDE solution, but an approximation of it, obtained by projecting the original discretized equations onto a well-chosen basis. In the application cases given above, however, one is not interested in the solution by itself, but rather in a *quantity of interest*, or model *output*, which is a functional of this solution. Taking this functional into account when performing the model reduction leads to a so-called *goal-oriented* method. For instance, goal-oriented basis choice procedures have been tried with success in the context of dynamical systems in [17, 4], where the basis is chosen so as to contain the modes that are relevant to accurately represent the output of interest, and in a general context in [1], where the basis is chosen so as to minimize the overall output error. All those papers showed that using an adapted basis could lead to a great improvement of reduction error. This paper is about goal-

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oriented error estimation, that is, the description of a rigorous and computable *error bound* between the model output and the reduced one. In [7], the output error bounds are computed by using an adjoint-based method, which involves the application of the RB method to an auxiliary (dual) problem in order to correct the output and to compute a goal-oriented error bound. This method, however, has the drawback of doubling offline *and online* computational times. In this paper, we propose a new goal-oriented error bound which does not require a doubled online computation time, and we show, in numerical examples, that this method, for a fixed computational budget, outperforms the adjoint-based error bound.

This paper is organized as follows: in the first part, we describe our output error bound and give its method of computation; in the second part, we see how to apply our error bound to certified sensitivity analysis studies; finally, the third and fourth parts present the numerical applications of our method.

1. Methodology.

1.1. Preliminaries. We begin by setting up the context of the reduced basis method for affine-parameterized linear partial differential equations presented in [7]. Our reference problem is the following: given a parameter tuple $\mu \in \mathcal{P} \subset \mathbb{R}^p$, find $u(\mu)$, the solution (in a discretized functional space X of finite dimension) of:

$$A(\mu)u(\mu) = f(\mu), \quad (1.1)$$

where $A(\mu)$ is a μ -dependent invertible square matrix of dimension $\dim X$, and $f \in X$; then compute the *output*:

$$s(\mu) = s(u(\mu)) \quad (1.2)$$

where $s : X \rightarrow \mathbb{R}$ is a linear form on X .

Problems such as (1.1) usually appear as discretizations of μ -parametrized linear partial differential equations (PDE); the X space is typically a finite element subspace (for instance, Lagrange P^1 finite elements), and $A(\mu)$ and f are given by Galerkin projection of the weak form of the PDE onto a suitable basis of X . The boundary conditions of the PDE are usually either encoded in X or in $A(\mu)$.

The dimension of the finite element subspace $\dim X$ is generally fairly large, so that the numerical computation of $u(\mu)$ from the inversion of $A(\mu)$ is expensive. The reduced basis aims at speeding up “many queries”, that is, the computation of $u(\mu)$ for all parameters $\mu \in \mathcal{P}_0$ where \mathcal{P}_0 is a finite but “large” subset of the parameter set \mathcal{P} . We suppose that $A(\mu)$ and $f(\mu)$ admit the following so-called affine decomposition [7]:

$$\forall \mu \in \mathcal{P}, \quad A(\mu) = \sum_{q=1}^Q \Theta_q(\mu)A_q, \quad f(\mu) = \sum_{q'=1}^{Q'} \gamma_{q'}(\mu)f'_{q'} \quad (1.3)$$

where $Q, Q' \in \mathbb{N}^*$, $\Theta_q : \mathcal{P} \rightarrow \mathbb{R}$ and $\gamma_{q'} : \mathcal{P} \rightarrow \mathbb{R}$ (for $q = 1, \dots, Q$, $q' = 1, \dots, Q'$) are smooth functions, A_q are square matrices of dimension $\dim X$ and $f'_{q'} \in X$.

We suppose that X is endowed with the standard Euclidean inner product: $\langle u, v \rangle = u^t v$, with associated norm $\|u\| = \sqrt{\langle u, u \rangle}$, and consider a subspace \tilde{X} of X , and a matrix Z whose columns are the components of a basis of \tilde{X} in a basis of X . This basis of \tilde{X} is called the

reduced basis in the sequel. We denote by $\tilde{u}(\mu)$ the components, in the reduced basis, of the solution of the Galerkin projection of (1.1) onto \tilde{X} , that is, the solution of:

$$Z^t A Z \tilde{u}(\mu) = Z^t f(\mu) \quad (1.4)$$

(where, for any matrix M , M^t is the transpose of M).

The many-query computation can then be split into two parts: the first part (usually called the “offline phase”), which is done only once, begins by finding a reduced subspace and its basis (this gives the Z matrix), then the Q parameter-independent matrices:

$$\tilde{A}_q = Z^t A_q Z, \quad q = 1, \dots, Q$$

and the Q' vectors:

$$\tilde{f}_{q'} = Z^t f_{q'}, \quad q' = 1, \dots, Q'$$

are computed and stored. In the second part (the “online phase”), we compute, for each value of the parameter μ :

$$\tilde{A}(\mu) = \sum_{q=1}^Q \Theta_q(\mu) \tilde{A}_q, \quad \tilde{f}(\mu) = \sum_{q'=1}^{Q'} \gamma_{q'}(\mu) \tilde{f}_{q'} \quad (1.5)$$

and solve for $\tilde{u}(\mu)$ satisfying:

$$\tilde{A}(\mu) \tilde{u}(\mu) = \tilde{f}(\mu). \quad (1.6)$$

The key point is that the operations in (1.5) and (1.6) are performed on vectors and matrices of size $\dim \tilde{X}$, and that the complexity of these operations is totally independent from the dimension of the underlying “truth” subspace X . In many cases, the smoothness of the map $\mu \mapsto u(\mu)$ allows to find (in a constructive way, ie., compute) \tilde{X} so that $\dim \tilde{X} \ll \dim X$ while keeping $\|u(\mu) - Z\tilde{u}(\mu)\|$ small, hence enabling significant computational savings.

The output $s(\mu)$ can also be approximated from $\tilde{u}(\mu)$ using an efficient offline-online procedure: let $l \in X$ be so that:

$$s(u) = \langle l, u \rangle \quad \forall u \in X;$$

in the offline phase we compute and store:

$$\tilde{l} = Z^t l$$

and in the online phase we take:

$$\tilde{s}(\mu) = \langle \tilde{l}, \tilde{u}(\mu) \rangle$$

as an approximation for $s(\mu)$.

Under additional coercivity hypothesis on A , the reduced basis method [7] also provides an efficient offline-online procedure for computing $\epsilon^u(\mu)$ so that the approximation can be *certified*:

$$\forall \mu \in \mathcal{P} \quad \|u(\mu) - Z\tilde{u}(\mu)\| \leq \epsilon^u(\mu).$$

The online procedure for the computation of $\epsilon(\mu)$ is also of complexity independent of $\dim X$.

This online error bound can in turn be used to provide a certification on the output:

$$\forall \mu \in \mathcal{P} \quad |s(\mu) - \tilde{s}(\mu)| \leq \underbrace{\|l\| \epsilon^u(\mu)}_{=: \epsilon^L(\mu)} \quad (1.7)$$

and this bound is clearly “optimal” amongst those depending on μ through $\epsilon^u(\mu)$ only. We call this bound the “Lipschitz” bound, and denote it by $\epsilon^L(\mu)$.

We here notice that [7] uses a different approximation of $s(\mu)$, which also depends on the solution of the adjoint equation of (1.1) projected on a suitably selected dual reduced basis. While this approximation has a better rate of convergence, its computation roughly requires doubling of both offline and online complexities as well as storage requirements. The aim of our work is to bound $|s(\mu) - \tilde{s}(\mu)|$ by a quantity which is smaller than the right-hand side of (1.7) and can be computed using an efficient offline-online procedure which does not require computation of $\epsilon^u(\mu)$ nor any adjoint problem solution during the online phase.

1.2. Theoretical error bound. In this section, we give the expression of our output error bound. We begin by some notations: let’s denote the residual by $r(\mu)$:

$$r(\mu) = A(\mu)Z\tilde{u}(\mu) - f(\mu) \in X,$$

and the adjoint problem solution (which will naturally appear in the proof of Theorem 1.1) by $w(\mu)$:

$$w(\mu) = A(\mu)^{-t}l.$$

Let, for any orthonormal basis $\Phi = \{\phi_1, \dots, \phi_N\}$ of X , any $N \in \mathbb{N}^*$, and $i = 1, \dots, N$,

$$D_i(\mu, \Phi) = \langle w(\mu), \phi_i \rangle.$$

We take a partition $\{\mathcal{P}_1, \dots, \mathcal{P}_K\}$ of the parameter space \mathcal{P} , that is:

$$\mathcal{P} = \cup_{k=1}^K \mathcal{P}_k \quad \text{and} \quad k \neq k' \rightarrow \mathcal{P}_k \cap \mathcal{P}_{k'} = \emptyset.$$

We set, for $i = 1, \dots, N$ and $k = 1, \dots, K$:

$$\beta_{i,k}^{min}(\Phi) = \min_{\mu \in \mathcal{P}_k} D_i(\mu), \quad \beta_{i,k}^{max}(\Phi) = \max_{\mu \in \mathcal{P}_k} D_i(\mu),$$

and:

$$\beta_i^{up}(\mu, \Phi) = \begin{cases} \beta_{i,k(\mu)}^{max}(\Phi) & \text{if } \langle r(\mu), \phi_i \rangle > 0 \\ \beta_{i,k(\mu)}^{min}(\Phi) & \text{else,} \end{cases}$$

$$\beta_i^{low}(\mu, \Phi) = \begin{cases} \beta_{i,k(\mu)}^{min}(\Phi) & \text{if } \langle r(\mu), \phi_i \rangle > 0 \\ \beta_{i,k(\mu)}^{max}(\Phi) & \text{else,} \end{cases}$$

where $k(\mu)$ is the only k in $\{1, \dots, K\}$ so that $\mu \in \mathcal{P}_k$. We also set:

$$T_1^{low}(\mu, N, \Phi) = \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \beta_i^{low}(\mu, \Phi), \quad T_1^{up}(\mu, N, \Phi) = \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \beta_i^{up}(\mu, \Phi),$$

$$T_1(\mu, N, \Phi) = \max \left(\left| T_1^{low}(\mu) \right|, \left| T_1^{up}(\mu) \right| \right).$$

Finally, we suppose that μ is a random variable on \mathcal{P} and set:

$$T_2(N, \Phi) = \mathbf{E}_\mu \left(\left| \sum_{i>N} \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle \right| \right),$$

where we take, for convenience, $\phi_i = 0$ for all $i > \mathcal{N}$ (so that the sum above is in fact between N and \mathcal{N}).

We have the following theorem:

Theorem 1.1. *For any $\alpha \in]0; 1[$ and for any $N \in \mathbb{N}^*$, we have:*

$$P \left(|s(\mu) - \tilde{s}(\mu)| > T_1(\mu, N, \Phi) + \frac{T_2(N, \Phi)}{\alpha} \right) \leq \alpha.$$

Proof: We begin by noticing that:

$$A(\mu)^{-1}r(\mu) = Z\tilde{u}(\mu) - u(\mu)$$

so that:

$$\tilde{s}(\mu) - s(\mu) = \langle l, Z\tilde{u}(\mu) - u(\mu) \rangle = \langle l, A(\mu)^{-1}r(\mu) \rangle = \langle w(\mu), r(\mu) \rangle$$

We expand the residual in the Φ basis:

$$r(\mu) = \sum_{i \geq 1} \langle r(\mu), \phi_i \rangle \phi_i.$$

Hence:

$$\tilde{s}(\mu) - s(\mu) = \sum_{i \geq 1} \langle l, A(\mu)^{-1} \phi_i \rangle \langle r(\mu), \phi_i \rangle = \sum_{i \geq 1} \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle. \quad (1.8)$$

We clearly have that for any $N \in \mathbb{N}^*$, :

$$\sum_{i=1}^N \langle r(\mu), \phi_i \rangle \beta_i^{low}(\mu, \Phi) \leq \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \langle w(\mu), \phi_i \rangle \leq \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \beta_i^{up}(\mu, \Phi)$$

and this implies:

$$\left| \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \langle w(\mu), \phi_i \rangle \right| \leq T_1(\mu, N, \Phi). \quad (1.9)$$

So we have:

$$\begin{aligned}
& P \left(|s(\mu) - \tilde{s}(\mu)| > T_1(\mu, N, \Phi) + \frac{T_2(N, \Phi)}{\alpha} \right) \\
& \leq P \left(|s(\mu) - \tilde{s}(\mu)| > \left| \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \langle A(\mu)^{-t} l, \phi_i \rangle \right| + \frac{T_2(N, \Phi)}{\alpha} \right) \text{ by (1.9)} \\
& = P \left(|s(\mu) - \tilde{s}(\mu)| - \left| \sum_{i=1}^N \langle r(\mu), \phi_i \rangle \langle A(\mu)^{-t} l, \phi_i \rangle \right| > \frac{T_2(N, \Phi)}{\alpha} \right) \\
& \leq P \left(\left| \sum_{i>N} \langle r(\mu), \phi_i \rangle \langle A(\mu)^{-t} l, \phi_i \rangle \right| > \frac{T_2(N, \Phi)}{\alpha} \right) \text{ by (1.8)} \\
& \leq \alpha \text{ thanks to Markov's inequality. } \blacksquare
\end{aligned}$$

Choice of Φ . The error bound given in Theorem 1.1 above is valid for any orthonormal basis Φ . For efficiency reasons, we would like to choose Φ so that the parameter-independent part $T_2(N, \Phi)$ is the smallest possible, for a fixed truncation index $N \in \mathbb{N}^*$.

To our knowledge, minimizing $T_2(N, \Phi)$ over orthonormal bases of X is an optimization problem for which no efficient algorithm exists. However, we can minimize an upper bound of $T_2(N, \Phi)$.

We define an auto-adjoint, positive operator $G : X \rightarrow X$ by:

$$\forall \phi \in X, \quad G\phi = \frac{1}{2} \mathbf{E}_\mu (\langle r(\mu), \phi \rangle r(\mu) + \langle w(\mu), \phi \rangle w(\mu)). \quad (1.10)$$

Let $\lambda_1 \geq \lambda_2 \geq \dots \lambda_{\mathcal{N}} \geq 0$ be the eigenvalues of G . Let, for $i \in \{1, 2, \dots, \mathcal{N}\}$, ϕ_i^G be a unit eigenvector of G associated with the i^{th} eigenvalue, and $\Phi^G = \{\phi_1^G, \dots, \phi_{\mathcal{N}}^G\}$.

We can state that:

Theorem 1.2.

$$T_2(N, \Phi^G) \leq \sum_{i>N} \lambda_i^2.$$

Proof. We have:

$$T_2(N, \Phi) \leq \frac{1}{2} \mathbf{E}_\mu \left(\sum_{i>N} \langle (\mu), \phi_i \rangle^2 + \sum_{i>N} \langle r(\mu), \phi_i \rangle^2 \right) =: T_2^{sup}(N, \Phi) = \sum_{i>N} \langle G\phi_i, \phi_i \rangle$$

Using Theorem 1.1 of [16], we get that the minimum of $T_2^{sup}(N, \Phi)$ is attained for $\Phi = \Phi^G$, and that minimum is $\sum_{i>N} \lambda_i^2$. \blacksquare

This theorem suggests to use $\Phi = \Phi^G$, so as to control $T_2(N, \Phi)$.

1.3. Computable error bound. In this Subsection, we present an implementable offline/online procedure for the estimation of the upper bound for $|\tilde{s}(\mu) - s(\mu)|$ presented in Theorem 1.1.

Estimation of ϕ_i^G . We fix a truncation index $N \in \mathbb{N}^*$, and we estimate $\{\phi_i^G\}_{i=1,\dots,N}$ by using a modification of the method of snapshots used in Proper Orthogonal Decomposition [13]. This estimation is performed during the offline phase. We take a finite (large), subset of parameters $\Xi \subset \mathcal{P}$, randomly sampled from the distribution of the parameter, and we approximate the G operator by:

$$\widehat{G}\phi = \frac{1}{2\#\Xi} \sum_{\mu \in \Xi} (\langle r(\mu), \phi \rangle r(\mu) + \langle w(\mu), \phi \rangle w(\mu))$$

In other words, \widehat{G} is a Monte-Carlo estimator of G . We take $\{\widehat{\phi}_i^G\}_{i=1,\dots,N}$ as the unit eigenvectors associated with the N largest eigenvalues of \widehat{G} .

The operator \widehat{G} admits the following matrix representation:

$$\widehat{G} = \frac{1}{2\#\Xi} (WW^t + RR^t),$$

where W (resp. R) is the matrix whose columns are the components of $w(\mu)$ (resp. $r(\mu)$) in a basis of X , for $\mu \in \Xi$. These two matrices have $\#\Xi$ columns and $\dim X$ lines, which means that the matrix above is $\dim X \times \dim X$. In general, we take $\#\Xi \ll \dim X$, and so it is computationally advantageous to notice that if ϕ is an eigenvector of \widehat{G} associated with a nonzero eigenvalue λ , then:

$$\frac{1}{\lambda} \frac{1}{2\#\Xi} ((WW^t\phi + RR^t\phi)) = \phi,$$

so that $\phi \in \text{Im } W + \text{Im } R =: \mathcal{V}$. Hence, if V is the matrix of an orthonormal basis of \mathcal{V} , then there exists ψ so that $\phi = V\psi$ and we have:

$$WW^t\phi + RR^t\phi = \lambda\phi \implies \left[V^t \frac{1}{2\#\Xi} ((WW^t + RR^t)) V \right] \psi = \lambda\psi.$$

As a consequence, it is sufficient to find the dominant eigenvectors $\widehat{\psi}_1^G, \dots, \widehat{\psi}_N^G$ of the matrix $\Sigma = \frac{1}{2\#\Xi} V^t (WW^t + RR^t) V$ (of size 2Ξ), and to deduce $\widehat{\phi}_i^G$ from $\widehat{\psi}_i^G$ by the relation $\widehat{\phi}_i^G = V\widehat{\psi}_i^G$. Besides, by writing Σ as:

$$\Sigma = \frac{1}{2\#\Xi} ((V^t W)(W^t V) + (V^t R)(R^t V)),$$

it is possible to compute and store Σ without storing nor computing any dense $\dim X \times \dim X$ matrix.

Computation of $T_1(\mu, N, \Phi)$. For $i = 1, \dots, N$ and $k = 1, \dots, K$, the reals $\beta_{i,k}^{min}(\Phi)$ and $\beta_{i,k}^{max}(\Phi)$ can be computed during the offline phase, as they are parameter-independent. They can be approximated by a simple discrete minimization:

$$\widetilde{\beta}_{i,k}^{min}(\Phi) = \min_{\mu \in \Xi \cap \mathcal{P}_k} D_i(\mu, \Phi), \quad \widetilde{\beta}_{i,k}^{max}(\Phi) = \max_{\mu \in \Xi \cap \mathcal{P}_k} D_i(\mu, \Phi),$$

or, thanks to the availability of the gradient of $D_i(\mu)$ with respect to μ , by a more elaborate quasi-Newton optimization such as L-BFGS [18].

We also compute the following parameter-independent, offline-computable quantities:

$$\langle f_{q'}, \widehat{\phi}_i^G \rangle, \langle A_q \zeta_j, \widehat{\phi}_i^G \rangle \quad (i = 1, \dots, N, j = 1, \dots, n, q = 1, \dots, Q, q' = 1, \dots, Q')$$

where $\{\zeta_1, \dots, \zeta_n\}$ is a basis of the reduced space \widetilde{X} .

Now, let a parameter $\mu \in \mathcal{P}$ be given, and let $\widetilde{u}_1(\mu), \dots, \widetilde{u}_n(\mu)$ be the components of the reduced solution $\widetilde{u}(\mu)$ in the reduced basis $\{\zeta_1, \dots, \zeta_n\}$.

By using the relation:

$$\langle r(\mu), \widehat{\phi}_i^G \rangle = \sum_{q=1}^Q \Theta_q(\mu) \sum_{j=1}^n \widetilde{u}_j(\mu) \langle A_q \zeta_j, \widehat{\phi}_i^G \rangle - \sum_{q'=1}^{Q'} \gamma_{q'}(\mu) \langle f_{q'}, \widehat{\phi}_i^G \rangle,$$

the dot products between the residual and $\widehat{\phi}_i^G$ can be computed in the online phase, with a complexity of $O(nQ + Q')$ arithmetic operations, $O(Q)$ evaluations of Θ functions and $O(Q')$ evaluations γ functions, which is independent of $\dim X$. Then, β_i^{low} and β_i^{up} can be straightforwardly deduced.

Estimation of $T_2(N, \Phi)$, final error bound. We approximate $T_2(N, \Phi)$ by computing the following Monte-Carlo estimator:

$$\widehat{T}_2(N, \Phi) = \frac{1}{2\#\Xi} \sum_{\mu \in \Xi} \left| \widetilde{s}(\mu) - s(\mu) - \sum_{i=1}^N \langle w(\mu), \phi_i \rangle \langle r(\mu), \phi_i \rangle \right|.$$

As this quantity is μ -independent, it can be computed once and for all during the offline phase.

By using Theorem 1.1, we get that for $\epsilon(\mu, \alpha, N, \Phi) = T_1(\mu, N, \Phi) + T_2(N, \Phi)/\alpha$, we have:

$$P(|s(\mu) - \widetilde{s}(\mu)| \geq \epsilon(\mu, \alpha, N, \Phi)) \leq \alpha,$$

so we may take, as estimated error bound with risk α ,

$$\widehat{\epsilon}(\mu, \alpha, N, \Phi) = T_1(\mu, N, \Phi) + \frac{\widehat{T}_2(N, \Phi)}{\alpha}. \quad (1.11)$$

2. Application to sensitivity analysis. Our error estimation method is applied in sensitivity analysis, so as to quantify the error caused by the replacement of the original model output by the reduced basis output during the Monte-Carlo estimation of the Sobol indices. For the sake of self-completeness, we briefly present the aim and the computation of these indices, and we refer to [12], [11] and [5] for details.

2.1. Definition of the Sobol indices. For $i = 1, \dots, p$, the i^{th} Sobol index of a function of p variables $s(\mu_1, \dots, \mu_p)$ is defined by:

$$S_i = \frac{\text{Var}(\mathbb{E}(s(\mu_1, \dots, \mu_p) | \mu_i))}{\text{Var}(s(\mu_1, \dots, \mu_p))}, \quad (2.1)$$

the variances and conditional expectation being taken with respect to a postulated distribution of the (μ_1, \dots, μ_p) input vector accounting for the uncertainty on the inputs' value. These indices are well defined as soon as $s \in L^2(\mathcal{P})$ and that $\text{Var}(s(\mu_1, \dots, \mu_p)) \neq 0$. When μ_1, \dots, μ_p are (stochastically) independent, the i^{th} Sobol index can be interpreted as the fraction of the variance of the output that is caused by the uncertainty on the i^{th} parameter μ_i . All the Sobol indices lie in $[0; 1]$; the closer to zero (resp., one) S_i is, the less (resp., the more) importance μ_i 's uncertainty has on s 's uncertainty.

2.2. Estimation of the Sobol indices. The conditional expectation and variances appearing in (2.1) are generally not amenable to analytic computations. In those cases, one can estimate S_i by using a Monte-Carlo method which works as follows: from two M -sized random, independent samples of inputs' distribution, we compute $2M$ appropriate evaluations $\{s_j\}$ and $\{s'_j\}$ of s , and estimate S_i by:

$$\widehat{S}_i = \frac{\frac{1}{M} \sum_{j=1}^M s_j s'_j - \left(\frac{1}{M} \sum_{j=1}^M s_j \right) \left(\frac{1}{M} \sum_{j=1}^M s'_j \right)}{\frac{1}{M} \sum_{j=1}^M s_j^2 - \left(\frac{1}{M} \sum_{j=1}^M s_j \right)^2}. \quad (2.2)$$

When M and/or the required time for the evaluation of the model output are large, it is computationally advantageous to replace s by its surrogate model \tilde{s} . By using (2.2) on \tilde{s} (hence with reduced model outputs $\{\tilde{s}_j\}$ and $\{\tilde{s}'_j\}$), one estimates the Sobol indices of the surrogate model rather than those of the true model. We presented in [5], Sections 3.1 and 3.2, a method to quantify the error made in the Sobol index estimation when replacing the original model by the surrogate one, we presented in [5], Sections 3.1 and 3.2, two estimators $\widehat{S}_{i,\alpha_{as}/2}^m$ and $\widehat{S}_{i,1-\alpha_{as}/2}^M$ relying on output error bound samples $\{\epsilon_j\}$ and $\{\epsilon'_j\}$ so that we have:

Theorem 2.1. *If:*

$$\forall j = 1, \dots, M, \quad |s_j - \tilde{s}_j| \leq \epsilon_j \quad \text{and} \quad |s'_j - \tilde{s}'_j| \leq \epsilon'_j,$$

then we have:

$$P \left(S_i \in [\widehat{S}_{i,\alpha_{as}/2}^m; \widehat{S}_{i,1-\alpha_{as}/2}^M] \right) \geq 1 - \alpha_{as}.$$

In our case, the output error bound $\epsilon(\mu)$ of Theorem 1.1 does not satisfy the above hypothesis, but satisfies a weaker ‘‘probabilistic’’ statement. This is the object of the following Corollary:

Corollary 2.2. *If:*

$$\forall j = 1, \dots, M, \quad P(|s_j - \tilde{s}_j| \geq \epsilon_j) \leq \alpha \quad \text{and} \quad \forall j = 1, \dots, M, \quad P(|s'_j - \tilde{s}'_j| \geq \epsilon'_j) \leq \alpha,$$

then we have:

$$P \left(S_i \in [\widehat{S}_{i,\alpha_{as}/2}^m; \widehat{S}_{i,1-\alpha_{as}/2}^M] \right) \geq (1 - \alpha_{as}) \times (1 - \alpha)^{2M}.$$

Proof. We easily have that:

$$\begin{aligned} P \left(S_i \in [\widehat{S}_{i,\alpha_{as}/2}^m; \widehat{S}_{i,1-\alpha_{as}/2}^M] \right) &\geq P \left(S_i \in [\widehat{S}_{i,\alpha_{as}/2}^m; \widehat{S}_{i,1-\alpha_{as}/2}^M] \mid \forall j, |s_j - \tilde{s}_j| < \epsilon(\mu) \right) \\ &\quad \times P(\forall j, |s_j - \tilde{s}_j| < \epsilon(\mu)) \\ &\geq (1 - \alpha_{as}) \times (1 - \alpha)^{2M}. \end{aligned}$$

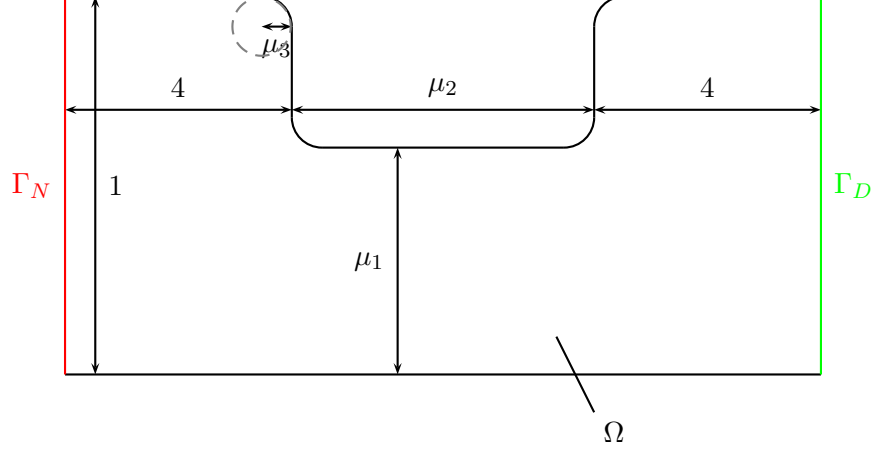
■

3. Numerical results I: Diffusion equation.

3.1. Benchmark problem. Our benchmark problem [10] is the following: given a parameter vector

$$\mu = (\mu_1, \mu_2, \mu_3) \in \mathcal{P} = [0.25, 0.5] \times [2, 4] \times [0.1, 0.2],$$

we consider the domain $\Omega = \Omega(\mu)$ below:



Our continuous field variable $u_e = u_e(\mu) \in X_e$ satisfies:

$$\begin{cases} \Delta u_e = 0 & \text{in } \Omega \\ u_e = 0 & \text{on } \Gamma_D \\ \frac{\partial u_e}{\partial n} = -1 & \text{on } \Gamma_N \\ \frac{\partial u_e}{\partial n} = 0 & \text{on } \partial\Omega \setminus (\Gamma_N \cup \Gamma_D) \end{cases} \quad (3.1)$$

where

$$X_e = \{v \in H^1(\Omega) \text{ s.t. } v|_{\Gamma_D} = 0\},$$

Δ denotes the Laplace operator, and $\frac{\partial}{\partial n}$ is the normal derivative with respect to $\partial\Omega$.

This continuous variable denotes the potential of a steady, incompressible flow moving in a tube whose profile is given by Ω , with open ends on Γ_N and Γ_D . The Neumann boundary condition on Γ_N states that the fluid enters by Γ_N with unit speed, the condition on $\partial\Omega \setminus (\Gamma_N \cup \Gamma_D)$ states that the velocity field is tangential to the boundary of the tube; finally the Dirichlet condition on Γ_D guarantees well-posedness, as the potential field is determined up to a constant.

The problem (3.1) is equivalent to the following variational formulation: find $u_e = u_e(\mu) \in X_e$ so that:

$$\int_{\Omega} \nabla u_e \cdot \nabla v = - \int_{\Gamma_N} v \quad \forall v \in X_e.$$

This variational problem is well-posed, as the bilinear form $(u, v) \mapsto \int_{\Omega} \nabla u \cdot \nabla v$ is coercive on X_e (see, for instance, [14], lemma A.14).

The above variational problem is discretized using a finite triangulation \mathcal{T} of Ω and the associated $P^1(\mathcal{T})$ (see [2] or [9]) finite element subspace: find $u \in X$ so that

$$\int_{\Omega} \nabla u \cdot \nabla v = - \int_{\Gamma_N} v \quad \forall v \in X,$$

where $X = \{v \in \mathbf{P}^1(\mathcal{T}) \text{ s.t. } v|_{\Gamma_D} = 0\}$.

In our experiments, $\dim X = 525$.

The affine decomposition of the matrix of the bilinear form in the left-hand side of the above equation is obtained by using a piecewise affine mapping from $\Omega(\mu)$ to a reference domain $\bar{\Omega}$ as explained in [8], page 11. The number of terms in the obtained affine decompositions are $Q = 9$ and $Q' = 1$.

Our scalar output of interest is taken to be:

$$s(\mu) = \int_{\Gamma_N} u(\mu),$$

and \mathcal{P} is endowed with the uniform distribution.

3.2. Results. We now present the numerical results obtained using our error estimation procedure on the output of the model described above. We give a comparison with the natural ‘‘Lipschitz’’ bound $\epsilon^L(\mu)$ given in (1.7) and with the dual-based error estimation method [7]. The bound $\epsilon^u(\mu)$ on $\|Z\tilde{u}(\mu) - u(\mu)\|$ is computed using the procedure described in [7]. Note that we estimated the ‘‘lower bound for the inf-sup parameter’’ ‘‘by inspection’’, as explained in [7], Section 3.3.2.

We also compare our goal-oriented error bound with the dual-based error bound method described in [7] (Section 3.2). This method involves the computation, during the online phase, of the reduced-basis solution of a linear, output-dependent, adjoint problem. The solution of this adjoint problem enables correction and estimation of the reduced output, at the expense of a doubled online computation cost.

For the comparisons to be fair, one should compare the error bounds of same online cost. It is widely assumed that there exists a constant C so that this cost is $C \times 2(\dim \tilde{X})^3$ for the dual-based method, and $C(\dim \tilde{X})^3$ for our method, since dual-based method involves online inversion of two linear systems of size $\dim \tilde{X}$, and one system of the same size for our method. Hence, the reported reduced basis sizes for the dual method are multiplied by a factor $\sqrt[3]{2}$.

In all cases, the reduced bases are computed using POD with snapshot size 80. To compute \hat{G} , we use a snapshot of size 200.

The partition used to split the \mathcal{P} set is compound of $K = 8$ cubes whose edges are parallel to the axes, and are chosen to contain (approximatively) the same number of points of an input sample.

In Figure 3.1, we give, for various reduced bases and various target risk levels α , the mean error bound on the output:

$$\bar{\epsilon} = \frac{1}{\#S} \sum_{\mu \in S} \hat{\epsilon}(\mu, \alpha, N, \Phi)$$

where S is a random subset of \mathcal{P} with size 200, $\hat{\epsilon}(\mu, \alpha, N, \Phi)$ is defined at (1.11), and the truncation index N is taken equal to 15.

For all the graphs, a unique test sample S is kept so as to guarantee fair comparisons.

Note that, due to limited numerical precision, the error bounds have been truncated upwards to 9×10^{-5} .

We observe that our new, goal-oriented, output error bound largely outperforms the non-goal-oriented Lipschitz bound and is better than the goal-oriented, dual-based error bound.

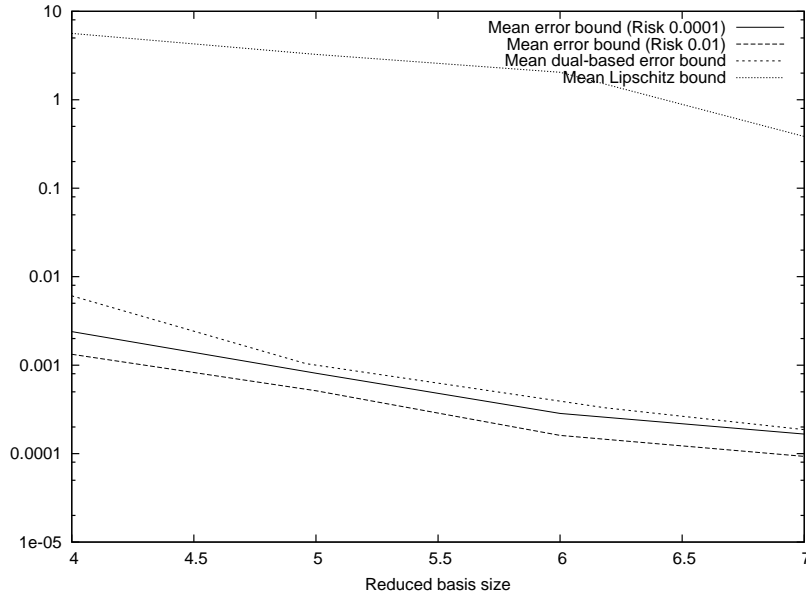


Figure 3.1. Comparison of the mean error bounds (for risk $\alpha \in \{0.01, 0.0001\}$), the mean Lipschitz bounds and the mean dual-based error bounds.

Finally, we observe that the high concentration of \widehat{T}_2 around zero allows us to choose a very low target risk and remain very competitive.

3.3. Application to sensitivity analysis. We estimate confidence intervals for the sensitivity indices of $s(\mu)$ by using the method described in [5], together with the remarks in Section 2.2.

We take $M = 1000$ as sample size, $B = 500$ as number of bootstrap replications, $\dim \tilde{X} = 10$ as reduced basis size, $\alpha = 0.00001$ as output error bound risk, and $\alpha_{as} = 0.05$ as Monte-Carlo risk. The level of the combined confidence interval $[\widehat{S}_{i,\alpha_{as}/2}^m; \widehat{S}_{i,1-\alpha_{as}/2}^M]$ is then $(1 - \alpha_{as})(1 - \alpha)^M > 0.93$.

The results are gathered in Table 3.1. The spread between \widehat{S}_i^m and \widehat{S}_i^M accounts for the *metamodel-induced* error in the estimation of the Sobol indices. The remaining spread between $\widehat{S}_{i,\alpha_{as}/2}^m$ and $\widehat{S}_{i,1-\alpha_{as}/2}^M$ is the impact of the sampling error (due to the replacement of the variances in the definition of the Sobol indices by their empirical estimators). We see that, in this case, the metamodel-induced error (certified by the use of our goal-oriented error bound) is very small with regard to the sampling error.

4. Numerical results II: transport equation. We now apply our error bound on a non-homogeneous linear transport equation. Compared to the previous example, the considered PDE is of a different kind (hyperbolic rather than elliptic).

4.1. Benchmark problem. In this problem, the continuous field $u_e = u_e(x, t)$ is the solution of the linear transport equation:

$$\frac{\partial u_e}{\partial t}(x, t) + \mu \frac{\partial u_e}{\partial x}(x, t) = \sin(x) \exp(-x)$$

Input parameter	$\widehat{S}_i^m; \widehat{S}_i^M$	$\widehat{S}_{i,\alpha_{as}/2}^m; \widehat{S}_{i,1-\alpha_{as}/2}^M$
μ_1	[0.530352;0.530933]	[0.48132; 0.5791]
μ_2	[0.451537;0.452099]	[0.397962;0.51139]
μ_3	[0.00300247;0.0036825]	[-0.0575764;0.0729923]

Table 3.1

Results of the application of Section 2 to the estimation of the Sobol indices of the output of our benchmark model.

for all $(x, t) \in]0, 1[\times]0, 1[$, satisfying the initial condition:

$$u_e(x, t = 0) = x(1 - x) \quad \forall x \in [0, 1],$$

and boundary condition:

$$u_e(x = 0, t) = 0 \quad \forall t \in [0, 1].$$

The parameter μ is chosen in $\mathcal{P} = [0.5, 1]$ and \mathcal{P} is endowed with the uniform measure.

We now choose a spatial discretization step $\Delta x > 0$ and a time discretization step $\Delta t > 0$, and we introduce our discrete unknown $u = (u_i^n)_{i=0,\dots,N_x;n=0,\dots,N_t}$ where

$$N_x = \frac{1}{\Delta x}, \quad \text{and} \quad N_t = \frac{1}{\Delta t}.$$

We note here that the considered PDE is hyperbolic and time-dependent, and that we perform the reduction on the space-time unknown u , of dimension $(N_x + 1) \cdot (N_t + 1)$. This is different from reducing the space-discretized equation at each time step.

The u vector satisfies the discretized initial-boundary conditions:

$$\forall i, \quad u_i^0 = (i\Delta x)(1 - i\Delta x) \quad (4.1)$$

$$\forall n, \quad u_0^n = 0 \quad (4.2)$$

and the first-order upwind scheme implicit relation:

$$\forall i, n \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} + \mu \frac{u_{i+1}^{n+1} - u_i^{n+1}}{\Delta x} = \sin(i\Delta x) \exp(-i\Delta x). \quad (4.3)$$

Let's denote by $B = B(\mu)$ (resp. y) the matrix (resp. the vector) so that (4.1),(4.2) and (4.3) are equivalent to:

$$Bu = y \quad (4.4)$$

that is:

$$B^T Bu = B^T y, \quad (4.5)$$

so that equation (4.5) is (1.1) with $A(\mu) = B^T B$ and $f = B^T y$.

The output of interest is: $s(\mu) = u_{N_x}^{N_t}$. In the following, we take $\Delta t = 0.02$ and $\Delta x = 0.05$.

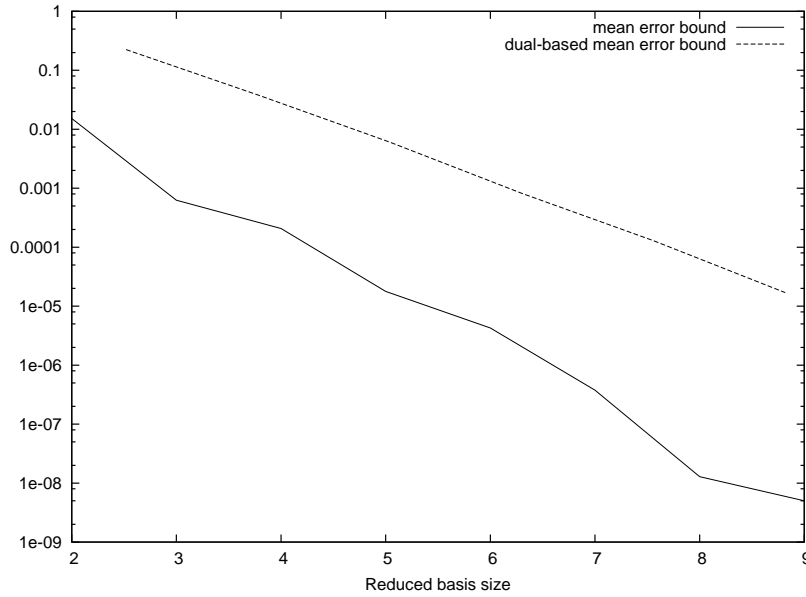


Figure 4.1. Comparison between the mean error bound (for risk $\alpha = 0.01$) and the mean dual-based error bound, for different reduced basis sizes.

4.2. Results. We took a very low risk level $\alpha = 0.0001$, a snapshot size of 70, $N = 10$ retained $\widehat{\phi}_i^G$ vectors and $K = 1$. The results (Figure 4.1) show that, once again, the error bound we propose in this paper outperforms the dual-based error bound.

Conclusion. We have presented a new explicitly computable output error bound for the reduced-basis method. We have shown, on two different practical examples, that this bound is clearly better than the naive Lipschitz bound and that, at the expense of a slight, controllable risk, the performances of this new bound are better than the existing dual-based output error bound.

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