



Numerical Analysis

Accurate a posteriori error evaluation in the reduced basis method

Évaluation précise de l'estimateur a posteriori dans la méthode des bases réduites

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ABSTRACT

In the reduced basis method, the evaluation of the a posteriori estimator can become very sensitive to round-off errors. In this Note, the origin of the loss of accuracy is revealed, and a solution to this problem is proposed and illustrated on a simple example.

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R É S U M É

Dans la méthode des bases réduites, l'évaluation de l'estimateur a posteriori peut s'avérer particulièrement sensible aux erreurs d'arrondis machine. Dans cette Note, l'origine de la perte de précision est révélée et une solution à ce problème est proposée et illustrée sur un exemple simple.

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1. Introduction

Consider the following discrete variational form, depending on a parameter $\mu \in \mathcal{P}$: find u_μ in a Hilbert space \mathcal{V} such that $\forall v \in \mathcal{V}$, $E_\mu: a_\mu(u_\mu, v) = b(v)$, where a_μ is a bilinear form and b a linear form. In a many queries context, a quantity of interest of the solution $q(u_\mu)$ has to be computed for many values of $\mu \in \mathcal{P}$. In this Note, the following assumptions are made for simplicity, but the conclusions are general: (i) the variational formulation is coercive, (ii) a_μ has a so-called affine dependence on the parameter μ so that $a_\mu = a_0 + \alpha_1(\mu)a_1$, (iii) the quantity of interest is the solution itself: $q(u_\mu) = u_\mu$.

Reduced basis (RB) strategies consist in replacing E_μ by an easily computable surrogate \hat{E}_μ , that is made precise below (see [2]). We denote \hat{u}_μ the solution of \hat{E}_μ , N the size of the matrix involved in the resolution of E_μ , and \hat{N} the size of the matrix involved in the resolution of \hat{E}_μ . The RB method consists in two steps: (i) An offline stage, where a basis, whose vectors are solutions of E_μ for well-chosen values of the parameter μ , is constructed using, e.g., a greedy algorithm on the parameter. During this stage, \hat{N} problems of size N are solved, and some quantities related to the solutions are stored. (ii) An online stage, where the precomputed quantities are used to solve \hat{E}_μ for many values of μ . In this stage, an a posteriori error estimator $\mathcal{E}(\mu)$ is also computed to check the quality of the approximation. This is called certification. The a posteriori error estimator verifies $\|u_\mu - \hat{u}_\mu\|_{\mathcal{V}} \leq \mathcal{E}(\mu) := \beta_\mu^{-1} \|G_\mu \hat{u}_\mu\|_{\mathcal{V}}$, where β_μ is the coercivity constant of a_μ (or a lower bound of it) and G_μ is the unique affine application from \mathcal{V} to \mathcal{V} such that $\forall (u, v) \in \mathcal{V}^2$, $(G_\mu u, v)_{\mathcal{V}} = a_\mu(u, v) - b(v)$. In this Note, we consider different ways to compute the same quantity $\mathcal{E}(\mu)$. We distinguish between formulae to compute $\mathcal{E}(\mu)$ by adding an index to $\mathcal{E}(\mu)$. Thus, $\mathcal{E}_1(\mu) := \beta_\mu^{-1} \|G_\mu \hat{u}_\mu\|_{\mathcal{V}}$ is the first formula for the estimator, directly given by

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the definition. Since $\mathcal{E}_1(\mu)$ requires the computation of a size N scalar product, this formula is not compatible with the constraint that the computations in the online stage should be of complexity independent of N .

Suppose that a reduced basis of size \hat{N} has been computed in the offline stage, namely a family $(\mu_i, u_i)_{i=1, \dots, \hat{N}}$, where each of the N -dimensional vectors u_i is the solutions of E_{μ_i} . The reduced problem is a Galerkin procedure on the u_i basis: find $\hat{u}_\mu \in \text{Span}\{u_1, \dots, u_{\hat{N}}\}$ such that $\forall j \in \{1, \dots, \hat{N}\}$, $\hat{E}_\mu: a_\mu(\hat{u}_\mu, u_j) = b(u_j)$. Writing $\hat{u}_\mu = \sum_{i=1}^{\hat{N}} \gamma_i(\mu) u_i$, the reduced linear system is $\hat{A}_\mu \hat{U}_\mu = \hat{b}$, where $(\hat{A}_\mu)_{i,j} = a_\mu(u_i, u_j)$, $(\hat{b})_j = b(u_j)$ and $(\hat{U}_\mu)_i = \gamma_i(\mu)$. Using the affine parameter dependence, the matrix $(\hat{A}_\mu)_{i,j} = a_0(u_i, u_j) + \alpha_1(\mu) a_1(u_i, u_j)$ is built and solved in complexity independent of N , provided that the quantities $a_0(u_i, u_j)$ and $a_1(u_i, u_j)$ have been precomputed in the offline stage.

Consider the Riesz isomorphism J from \mathcal{V}' to \mathcal{V} such that $\forall l \in \mathcal{V}'$, $\forall u \in \mathcal{V}$, $(Jl, u)_\mathcal{V} = l(u)$. The operator G_μ inherits the affine dependence of a_μ in μ since, $\forall u \in \mathcal{V}$,

$$G_\mu u = -Jb(\cdot) + Ja_0(u, \cdot) + \alpha_1(\mu) Ja_1(u, \cdot) =: G_{00} + G_0 u + \alpha_1(\mu) G_1 u, \quad (1)$$

where $b(\cdot)$ and $a_k(u, \cdot)$, $k \in \{0, 1\}$, are elements of \mathcal{V}' . The a posteriori error estimator is then written in the following compact form:

$$\mathcal{E}_2(\mu) := \beta_\mu^{-1} (\delta^2 + 2s^t x_\mu + x_\mu^t S x_\mu)^{\frac{1}{2}}, \quad (2)$$

where $\delta = \|G_{00}\|_\mathcal{V}$, $s_l = (G_{00}, G_k u_i)_\mathcal{V}$, $x_{\mu_l} = \alpha_k(\mu) \gamma_i(\mu)$, $S_{l,j} = (G_k u_i, G_l u_j)_\mathcal{V}$ (with l and j re-indexing respectively (k, i) and (l, j)), $0 \leq k, l \leq 1$, $1 \leq i, j \leq \hat{N}$ and $\alpha_0 = 1$. Provided that $\delta \in \mathbb{R}$, $s \in \mathbb{R}^{2\hat{N}}$, and $S \in \mathbb{R}^{2\hat{N} \times 2\hat{N}}$ (which are independent of μ) have been precomputed in the offline stage, $\mathcal{E}_2(\mu)$ is computed in complexity independent of N . This is what is typically used in RB implementations.

2. Round-off errors and certification

Canuto, Tonn and Urban [1] identified that the evaluation of $\mathcal{E}_2(\mu)$ suffers in practice from a loss of accuracy, which they attributed to the square root in (2). Herein, we show more precisely that this loss of accuracy comes from round-off errors. Indeed, when subtracting two real numbers within floating point arithmetics, the number of lost significant digits equals the number of common decimals between the two reals. For simplicity, we neglect the round-off errors introduced when solving E_μ and \hat{E}_μ , so that the vectors of the reduced basis u_i and the reduced solutions \hat{u}_μ are considered free of round-off errors. Therefore, we only consider round-off errors in the evaluation of $\mathcal{E}_1(\mu)$ and $\mathcal{E}_2(\mu)$ due to the summations. We define the machine precision ϵ by the maximal floating point representation relative error of real numbers: $|\frac{fl(x)-x}{x}| \leq \epsilon$. Under these hypotheses, the smallest possible values that can be practically computed for $\mathcal{E}_1(\mu)$ and $\mathcal{E}_2(\mu)$ using floating point arithmetics with machine precision ϵ is bounded below by respectively $\frac{\delta}{\beta_\mu} \epsilon$ and $\frac{\delta}{\beta_\mu} \sqrt{\epsilon}$. This is supported numerically (see Section 4).

This observation is of paramount importance since the certification of a RB procedure cannot be better than these values. In a successful RB procedure, the value of the estimator gets smaller as the size \hat{N} of the reduced basis increases. Enriching the basis with a new vector improves the quality of the approximation introduced by the method. As a result, there exists \hat{N}_0 such that, $\forall \hat{N} \geq \hat{N}_0$, $\forall \mu \in \mathcal{P}$, $\mathcal{E}(\mu) \leq \frac{\delta}{\beta_\mu} \sqrt{\epsilon}$. If $\hat{N} \geq \hat{N}_0$, $\mathcal{E}_2(\mu)$ is no longer suitable for computing the a posteriori error estimator.

We notice that increasing the machine precision from ϵ to ϵ^2 enables the accuracy of $\mathcal{E}_2(\mu)$ to reach the one of $\mathcal{E}_1(\mu)$. Thus, the use of quadruple precision is a first solution, checked numerically in Section 4. This is however not practical since current computer architectures are optimized for double precision. Another solution is to develop an alternative algorithm for the evaluation of the estimator that still achieves the machine precision. This is the purpose of the next section.

3. The new procedure for a posteriori error evaluation

Consider that a reduced basis of size \hat{N} has been constructed. Let us denote $d = 1 + 3\hat{N} + 2\hat{N}^2$. For a given μ and $\hat{u}_\mu \in \text{Span}\{u_1, \dots, u_{\hat{N}}\}$, we define $X(\mu) \in \mathbb{R}^d$ as the vector with components $(1, x_{\mu_1}, x_{\mu_1} x_{\mu_j})$, with $1 \leq l \leq j \leq 2\hat{N}$. Using the symmetry of the matrix S , we can write the right-hand side of (2) as a linear form in $X(\mu)$: $\sum_{p=1}^d q_p X_p(\mu)$, where q_p is independent of μ and $X_p(\mu)$ is the p -th component of $X(\mu)$.

During the offline stage, we take d values, possibly random, μ_r , $r \in \{1, \dots, d\}$, of the parameter μ . Then, we compute the vectors $X(\mu_r)$ and, using the accurate formula \mathcal{E}_1 for the estimator, the quantities $V_r := (\beta_{\mu_r} \mathcal{E}_1(\mu_r))^2$. Finally, we define $T \in \mathbb{R}^{d \times d}$ as the matrix whose columns are formed by the vectors $X(\mu_r)$ and we assume that T is invertible, which was the case in our simulations.

In the online stage, suppose that we want to evaluate the estimator for the parameter value μ . We compute the vector $X(\mu)$ and solve the linear system $T\lambda(\mu) = X(\mu)$, for $\lambda(\mu) \in \mathbb{R}^d$. We then have $X(\mu) = \sum_{r=1}^d \lambda_r(\mu) X(\mu_r)$ and

$$\sum_{p=1}^d q_p X_p(\mu) = \sum_{p,r=1}^d q_p \lambda_r(\mu) X_p(\mu_r) = \sum_{r=1}^d \lambda_r(\mu) (\beta_{\mu_r} \mathcal{E}_1(\mu_r))^2 = \sum_{r=1}^d \lambda_r(\mu) V_r. \quad (3)$$

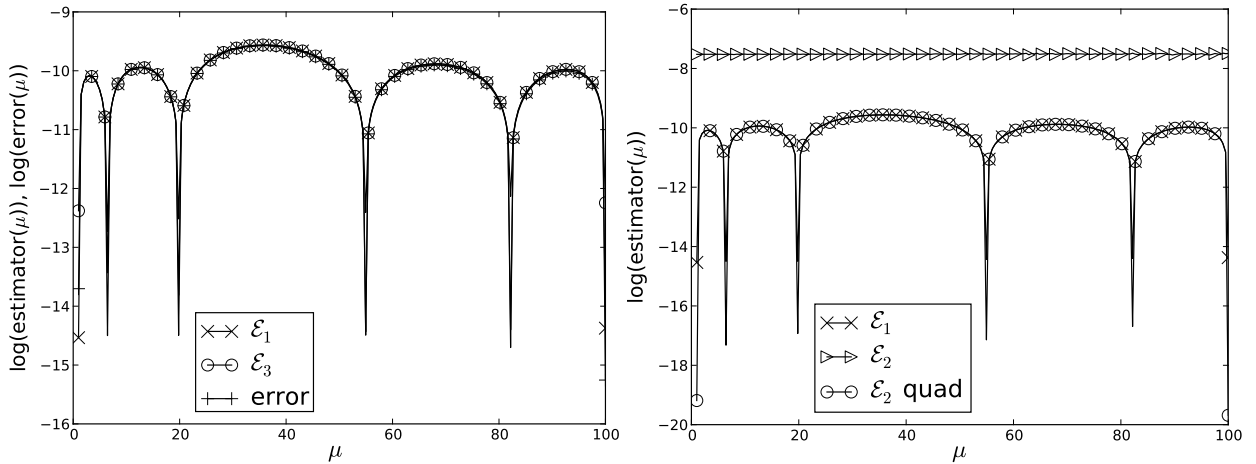


Fig. 1. Left: \mathcal{E}_1 , \mathcal{E}_3 algorithms for the estimator and error curves with respect to the parameter μ ; Right: \mathcal{E}_1 , \mathcal{E}_2 (double and quadruple precision) curves.

This yields the new formula for computing the estimator,

$$\mathcal{E}_3(\mu) := \beta_\mu^{-1} \left(\sum_{r=1}^d \lambda_r(\mu) V_r \right)^{\frac{1}{2}}. \tag{4}$$

Quite importantly, we notice that the additional cost is such that the quantity $\mathcal{E}_3(\mu)$ is still computed in complexity independent of N .

The quantity $(\beta_\mu \mathcal{E}_2(\mu))^2$ is a sum of terms, whose first one is fixed and equals δ^2 . On the contrary, $(\beta_\mu \mathcal{E}_3(\mu))^2$ is a sum whose terms V_r are updated each time a vector is added to the reduced basis. Since V_r is computed for $\mu_r \in \mathcal{P}$, $(\beta_\mu \mathcal{E}(\mu))^2$ and V_r (or, at least, $\max_{\mu \in \mathcal{P}} (\beta_\mu \mathcal{E}(\mu))^2$, and $\max_{1 \leq r \leq d} V_r$, which are the important quantities in a greedy selection and online certification) are of the same orders of magnitude.

4. Numerical illustration

Consider the equation $-u'' + \mu u = 1$ on $]0, 1[$ with $u(0) = u(1) = 0$, where $\mu \geq 1$ is the parameter. The analytic solution is

$$u(x) = -\frac{1}{\mu} (\cosh(\sqrt{\mu}x) - 1) + \frac{\cosh(\sqrt{\mu}) - 1}{\mu \sinh(\sqrt{\mu})} \sinh(\sqrt{\mu}x).$$

The Lax–Milgram theory is valid, the coercivity constant is 1 in the H^1 -norm. The estimator is given by $\mathcal{E}(\mu) = \|G_\mu \hat{u}_\mu\|_{H^1(]0,1])}$. Lagrange P_1 finite elements are used, with uniform mesh cells of length 0.005. The RB method is carried-out until a reduced basis of size 6 is constructed.

On the left part of Fig. 1, \mathcal{E}_3 yields the same curve as the accurate but expensive \mathcal{E}_1 algorithm. Notice that the values of the a posteriori error estimators are very close to the values of the error. This means that the efficiency of the estimator is very close to 1. On the right part of Fig. 1, we see that \mathcal{E}_2 yields a flat curve for the estimator, meaning that all information relative to the error is lost. As expected, the use of quadruple precision enables \mathcal{E}_2 to recover the accuracy levels of \mathcal{E}_1 . In this example, $\frac{\epsilon_\delta}{\beta} \approx 3 \times 10^{-17}$ and $\frac{\sqrt{\epsilon_\delta}}{\beta} \approx 3 \times 10^{-9}$, which should be respectively compared to the numerical values of \mathcal{E}_2 in quadruple precision and \mathcal{E}_1 (10^{-17} and 10^{-15}) and \mathcal{E}_2 (10^{-8}).

5. Conclusion

To sum up, we have developed a procedure where the accuracy of the online evaluation is limited by the accuracy of the evaluation of quantities precomputed during the offline stage, where heavy but accurate algorithms are allowed. In the online stage, instead of a linear combination of d terms, we have to solve a linear system of size d , before doing a linear combination of the same size. We have increased the accuracy of the estimator, with a procedure of complexity independent of the size N of the initial problem. When the size of the reduced basis increases, we observe that the condition number of the matrix T increases as well. Finally, we notice that oversampling strategies consisting in defining a least squares problem to compute $\lambda(\mu)$ such that T is rectangular with more than d columns improve the quality of our results when the RB is close to convergence. Experiments on a more complicated problem (external acoustics solved by integral equations where the criterion is on the far field approximation of the diffracted acoustic potential) lead to similar conclusions, which will be discussed in more detail elsewhere.

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