An overview of blackbox reduced-basis output bound methods for elliptic partial differential equations

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Abstract

We present a two-stage off-line/on-line blackbox reduced-basis output bound method for the prediction of outputs of interest of elliptic partial differential equations with affine parameter dependence. The computational complexity of the on-line stage of the procedure scales only with the dimension of the reduced-basis space and the parametric complexity of the partial differential operator. The method is both efficient and certain: thanks to rigorous a posteriori error bounds, we may retain only the minimal number of modes necessary to achieve the prescribed accuracy in the output of interest. The technique is particularly appropriate for applications such as design, optimization, and control, in which repeated and rapid evaluation of the output is required. In this paper three versions of this method are presented: (i) for coercive equilibrium problems, (ii) for symmetric eigenvalue problems, and (iii) for non-coercive equilibrium problems.

Key words: output bounds, reduced-basis techniques, a posteriori error estimation, partial differential equations.

AMS subject classifications: 65N15, 65N25, 65N30, 65F10.

1 Introduction

Reduced-basis methods [1, 7, 8] — projection onto low-order approximation spaces comprising solutions of the problem of interest at selected points in the parameter/design space — are efficient techniques for the prediction of linear functional outputs. These methods enjoy an optimality property which ensures rapid convergence even in high-dimensional parameter spaces; good accuracy may be obtained even with very few modes (basis functions), and thus the computational cost is typically very small.

It is often the case that the parameter enters affinely in the differential operator. This allows us to separate the computational steps into two stages: (i) the off-line stage, in which the reduced-basis space is constructed; and (ii) the on-line/real time stage, in which for each new parameter value the reduced-basis approximation for the output of interest is calculated. The on-line stage is "blackbox" in the sense that there is no longer any reference to the original problem formulation: the computational complexity of this stage scales only with the dimension of the reduced-basis space and the parametric complexity of the partial differential operator.

Although a priori theory [12] suggests the optimality of the reduced-basis space approximation, for a particular choice of the reduced-basis space the error in the output of interest is typically not known, and hence the minimal number of basis functions required to satisfy the desired error tolerance can not be ascertained. As a result, either too many or too few basis functions are retained; the former results in computational inefficiency, the latter in uncertainty and unacceptably inaccurate predictions. In this paper we review blackbox a posteriori methods [9] to address these shortcomings. In Section 2, we consider coercive equilibrium problems [5]; in Section 3, symmetric eigenvalue problems [3]; and in Section 4, non-coercive equilibrium problems [6].

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$\mathbf{2}$ Coercive Equilibrium Problems

2.1 **Preliminaries**

Let Y be a Hilbert space with an associated inner product $(\cdot,\cdot)_Y$ and an induced norm $\|\cdot\|_Y$. We define our parameter space to be $\mathcal{D} \subset \mathbb{R}^P$; a point in that space is denoted μ . Our problem is then to find $u \in Y$ such that

(1)
$$a(u, v; \mu) = \ell(v), \ \forall v \in Y,$$

and subsequently the output of interest $s(u) = \ell^O(u)$; $\ell(\cdot)$ and $\ell^O(\cdot)$ are both in Y', the dual space of Y. The bilinear form $a(\cdot,\cdot;\mu)$ is assumed to be symmetric, $a(w,v;\mu)=a(v,w;\mu)$, $\forall w,v\in Y$, and coercive, $\exists \ c>0$ such that $a(v,v;\mu) \geq c||v||_Y^2 > 0$, $\forall v \in Y$. Associated with the above primal problem we define the adjoint or dual problem for $\psi \in Y : a(v, \psi; \mu) = -\ell^{O}(v), \ \forall v \in Y.$ The need for this problem will become clear in the error estimation part.

We next choose a symmetric positive definite form $\hat{a}(w,v)$, and define $\lambda_{\hat{a}}^{1}(\mu)$ to be the minimum eigenvalue of $a(\varphi,v;\mu)=\lambda(\mu)\hat{a}(\varphi,v), \ \forall v\in Y.$ A lower bound for this eigenvalue is required by the output bound procedure: we assume that a $g(\mu)$ is known such that

(2)
$$a(v, v; \mu) \ge g(\mu)\hat{a}(v, v) > 0, \ \forall v \in Y \text{ and } \forall \mu \in \mathcal{D};$$

thus $g(\mu)$ is the required lower bound. It is also possible to include approximation of $\lambda_{\hat{a}}^1(\mu)$ as part of the reduced basis approximation [6].

Finally, for the blackbox method, we shall assume that, for some finite integer Q, there exists a decomposition of $a(w, v; \mu)$ of the form

(3)
$$a(w, v; \mu) = \sum_{q=1}^{Q} \sigma^{q}(\mu) a^{q}(w, v), \forall w, v \in Y \text{ and } \forall \mu \in \mathcal{D},$$

where we make no assumptions on the a^q other than bilinearity.

2.2 Reduced-Basis Approximation

We choose N/2 points in our parameter space \mathcal{D} , and form the sample set $S_N = \{\mu_1, \dots, \mu_{N/2}\}$. The reducedbasis spaces associated with the primal and dual problems are then given by $W_N^{pr} = \operatorname{span}\{u(\mu_1), \dots, u(\mu_{N/2})\}$ and $W_N^{du} = \operatorname{span}\{\psi(\mu_1), \dots, \psi(\mu_{N/2})\}$ respectively; we can then form

(4)
$$W_N = \text{span}\{u(\mu_1), \psi(\mu_1), \dots, u(\mu_{N/2}), \psi(\mu_{N/2})\} \equiv \text{span}\{\zeta_1, \dots, \zeta_N\}.$$

The space W_N defined this way has good approximation properties both for the primal and the dual problems.

For each new desired $\mu \in \mathcal{D}$, we now apply a standard Galerkin procedure over W_N to obtain $u_N(\mu)$ and $\psi_N(\mu)$ according to $a(u_N(\mu), v; \mu) = \ell(v), \ \forall v \in W_N$, and $a(v, \psi_N(\mu); \mu) = -\ell^O(v), \ \forall v \in W_N$. The output can then be calculated as $s_N(\mu) = \ell^O(u_N(\mu))$.

2.3**Bound Calculation**

We start by defining the residuals associated with the primal and dual reduced-basis approximations, $R_N^{pr}(v;\mu) =$ $\ell(v) - a(u_N(\mu), v; \mu), \ \forall v \in Y, \ \text{and} \ R_N^{du}(v; \mu) = -\ell^O(v) - a(v, \psi_N(\mu); \mu), \ \forall v \in Y, \ \text{respectively.}$ The Riesz representations $\hat{e}_N^{pr}(\mu)$ and $\hat{e}_N^{du}(\mu)$ of the primal and dual residual can then be defined as $\hat{a}(\hat{e}_N^{pr}(\mu), v) = R_N^{pr}(v; \mu), \ \forall v \in Y$ $Y, \ \hat{a}(\hat{e}_N^{du}(\mu), v) = R_N^{du}(v; \mu), \forall v \in Y.$

We then define, as in [3, 6],

$$\bar{s}_{N} = s_{N}(\mu) - \frac{1}{2g(\mu)} \hat{a}(\hat{e}_{N}^{pr}(\mu), \hat{e}_{N}^{du}(\mu))$$

$$\Delta_{N} = \frac{1}{2g(\mu)} \hat{a}^{1/2}(\hat{e}_{N}^{pr}(\mu), \hat{e}_{N}^{pr}(\mu)) \hat{a}^{1/2}(\hat{e}_{N}^{du}(\mu), \hat{e}_{N}^{du}(\mu)) ,$$
(5)

and compute lower and upper estimators $s_N^{\pm} = \bar{s}_N \pm \Delta_N$. It can be shown [3, 6] that s_N^+ (respectively s_N^-) will be an upper (respectively lower) bound for s provided that $g(\mu)$ is a lower bound for the eigenvalue $\lambda_{\hat{a}}^{1}(\mu)$ (or equivalently satisfies (2)). Note that in the general case, in which an \hat{a} , $g(\mu)$ which satisfy (2) are not readily available and an approximation to $\lambda_{\hat{a}}^{1}(\mu)$ must be computed as part of the

reduced-basis approximation, W_N must be augmented with eigenmodes corresponding to the minimum eigenvalue of the problem $a(\varphi, v; \mu) = \lambda(\mu)\hat{a}(\varphi, v), \ \forall v \in Y$ [6].

Also of interest is the quality of the bounds — how well they approximate the actual error. We measure the quality of the bounds by the effectivity $\eta_N(\mu)$, defined as the ratio of the bound gap Δ_N to $|s-\overline{s}_N|$. From the bound result we know that $\eta_N(\mu) \geq 1$. We can further prove that $\eta_N(\mu)$ is bounded independent of N; in practice, $\eta_N(\mu)$ is typically O(10), as desired.

2.4 Blackbox Method

The parametric dependence assumed in (3) permits us to decouple the computation into two stages: the off-line stage, in which (i) the reduced basis is constructed and, (ii) the necessary error-estimation preprocessing is performed; and the on-line stage, in which for each new desired value of μ , we compute $s_N(\mu)$ and the bounds. The essential "enablers" are the absence of μ dependence in \hat{a} and the affine dependence on μ of a, which allow us to precompute (and later assemble) all the "pieces" of $\hat{e}_N^{pr}(\mu)$, $\hat{e}_N^{du}(\mu)$ by linear superposition. A summary of the blackbox technique follows; see also [5].

In the off-line stage, we first form the reduced-basis stiffness matrices associated with each of the bilinear forms a^q, A^q . Next, we form error function "components": we recognize that R_N^{pr} and R_N^{du} are bilinear in μ and ζ_i , and we associate with each product term a "Green's" or influence function. These influence functions are inserted into the \hat{a} bilinear forms of (5) such that these error expressions can now be expressed as sums over N and Q appropriately weighted by the σ^q and the components of the reduced-basis solution vector. The computational complexity is NQ + N + 2 Y-linear system solves; $N^2Q^2 + 2NQ + 3$ \hat{a} -inner products, and 2N evaluations of linear functionals. In the on-line stage we first assemble the reduced-basis stiffness matrix A from the A^q ; this permits us to obtain the primal and dual reduced-basis solution vectors. These solution vectors, together with the σ_q , then allow us to construct the bound average and bound gap by appropriately summing the inner products precomputed in the off-line stage. For each new μ , the on-line stage requires $O(N^2Q^2 + N^3)$ operations to obtain the reduced-basis solution and bounds. Since $\dim(W_N) \ll \dim(Y)$, the cost to compute the reduced-basis output approximation and the corresponding upper and lower bounds will typically be much less than the direct evaluation of the output $s(\mu) = \ell^O(u(\mu))$ from (1).

2.5 Numerical Results

To illustrate our method we consider the thermal fin of Figure 1. The *i*th "radiator" of the fin has thermal conductivity k_i (normalized relative to the conductivity of the central post); and the fluid surrounding the fin is characterized by a heat convection coefficient expressed in nondimensional form by a Biot number, Bi. The fin geometry is described by the radiator length β and thickness α , both nondimensionalized with respect to the width of the fin base. We thus obtain P = 7, with a typical point in $\mathcal{D} \in \mathbb{R}^7$ given by $\mu = \{k_1, k_2, k_3, k_4, Bi, \alpha, \beta\}$. The output of interest is the average temperature over the fin base, Γ_1 .

In [5] we describe how this conduction problem can be readily cast in the form required by Section 2; we reproduce here a convergence analysis. In particular, we choose the design space $\mathcal{D} = [0.1, 10]^4 \times [0.01, 1.] \times [0.1, 0.5] \times [2.0, 3.0]$, and for μ the value $\{0.4, 0.6, 0.8, 1.2, 0.1, 0.3, 2.8\}$. To form the reduced space we choose N points randomly in \mathcal{D} . As we can see from Table 1, even for small N the accuracy is very good; furthermore, convergence with N is quite rapid. This is particularly noteworthy given the high-dimensional parameter space; even with N=50 points we have less than two points (effectively) in each parameter coor-

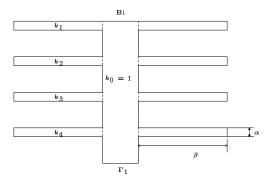


Figure 1

N	Δ_N	η_N
10	1.5987×10^{-1}	6.0211
20	1.5691×10^{-2}	6.6476
30	2.4267×10^{-3}	7.2929
40	7.2616×10^{-4}	8.4002
50	3.0620×10^{-4}	8.5741

Table 1

dinate. We also note that the effectivity remains roughly constant and O(10) with increasing N: the estimators are not only bounds, but relatively sharp bounds — good predictors for when N is "large enough." The behavior we observe at this particular value of μ is representative of most points in (a random sample over) \mathcal{D} , however there can certainly be points where the error or effectivity is large: more systematic study is required. In [5] we consider the application of this reduced-basis model to several problems in shape optimization.

3 The Symmetric Eigenvalue Problem

3.1 Problem Statement

Given our Hilbert space Y, we consider the symmetric eigenvalue problem [2]: find $(u, \lambda) \in Y \times \mathbb{R}$ such that

(6)
$$a(u, v; \mu) = \lambda m(u, v), \forall v \in Y, \text{ and } m(u, u) = 1,$$

where $\mu \in \mathcal{D}$ is any point in the design space, and $a(w,v;\mu)$, m(w,v) are symmetric bilinear forms; furthermore, we assume that $a(w,v,\mu)$ and m(w,v) are coercive and continuous in Y (see Section 2.1). In what follows, $0 < \lambda^1(\mu) \le \lambda^2(\mu) \le \ldots$ and $u^1(\mu), u^2(\mu), \ldots$ denote respectively the eigenvalues and eigenfunctions of (6) at $\mu \in \mathcal{D}$. For clarity, we suppose that the output of interest is the first eigenvalue $\lambda^1(\mu)$; we further assume that $\lambda^1(\mu) < \lambda^2(\mu)$. For this choice of output the definition of an adjoint problem is not required. This particular case, denoted compliance, leads to considerable simplification of the numerical procedure.

3.2 Reduced-Basis Approximation

We select the sample set $S_N = \{\mu_1, \dots, \mu_{N/2}\}$, and compute $u^1(\mu_i)$ and $u^2(\mu_i)$, $i = 1, \dots, N/2$. The reduced-basis space is then defined as

(7)
$$W_N \equiv \operatorname{span}\{u^1(\mu_1), u^2(\mu_1), \dots, u^1(\mu_{N/2}), u^2(\mu_{N/2})\} \equiv \operatorname{span}\{\zeta_1, \dots, \zeta_N\}.$$

Including the eigenfunctions corresponding to the second smallest eigenvalue permits the accurate prediction, by the reduced-basis approximation, of the second eigenpair at each point $\mu \in \mathcal{D}$. This in turn permits accurate prediction of the parameter β_N (defined in the next Section) required for the calculation of the bounds.

For each new desired $\mu \in \mathcal{D}$, the reduced-basis approximation can be obtained by Galerkin projection, $a(u_N(\mu), v; \mu) = \lambda_N(\mu) m(u_N(\mu), v)$, $\forall v \in W_N$; we denote by $(u_N^i(\mu), \lambda_N^i(\mu)) \in (W_N \times \mathbb{R})$, i = 1, 2, the first two eigenpairs, respectively.

3.3 Bound Calculation

We suppose a symmetric coercive bilinear form \hat{a} and a function $g(\mu)$ which satisfies (2). We start by defining the residual for the reduced-basis approximation as $R_N(v; u_N^1(\mu), \lambda_N^1(\mu); \mu) = \lambda_N^1(\mu) m(u_N^1(\mu), v) - a(u_N^1(\mu), v; \mu), \ \forall v \in Y$. The Riesz representation of the residual can then be computed as $\hat{a}(\hat{e}_N(\mu), v) = R_N(v; u_N^1(\mu), \lambda_N^1(\mu); \mu), \ \forall v \in Y$. Finally, the upper and lower bounds may be evaluated as

(8)
$$\lambda_{N}^{+}(\mu) = \lambda_{N}^{1}(\mu) \lambda_{N}^{-}(\mu) = \lambda_{N}^{1}(\mu) - \frac{1}{\beta_{N}g(\mu)} \hat{a}(\hat{e}_{N}(\mu), \hat{e}_{N}(\mu)) \equiv \lambda_{N}^{1} - 2\Delta_{N} ,$$

where, for some positive γ , $\beta_N \equiv 1 - \gamma - \lambda_N^1(\mu)/\lambda_N^2(\mu)$ is a positive parameter [3].

Due to the nonlinearity of the eigenvalue problem there are some higher order terms in the error expression; however thanks to certain general properties of Galerkin approximation of eigenvalue problems [2], our choice of β_N ensures that these terms are asymptotically strictly dominated by the positive-definite terms [3]. The bounds calculated by (8) are thus asymptotic; $\lambda_N^-(\mu) \leq \lambda_N^+(\mu)$, $\forall N \geq N^*(\mu)$ for some N^* .

3.4 Blackbox Formulation and Numerical Results

Assuming that a decomposition of the form (3) exists, then a blackbox formulation is again possible [3]. As a test case, we reconsider our fin problem, but we now compute as output the minimum eigenvalue; the results are presented in Table 2, for $\mathcal{D} = [0.1, 10]^4 \times [0.01, 1.] \times [0.25, 0.25] \times [2.5, 2.5]$, and $\mu = \{0.2, 0.9, 3, 9, 0.6, 0.25, 2.5\}$. We observe very fast convergence with increasing N; furthermore the effectivity, η_N , is O(10)—the error bars are relatively tight. Note also that $N^*(\mu) = 1$: bounds are obtained in all cases.

Ν	Δ_N	η_N
10	9.46×10^{-2}	5.63
20	1.02×10^{-2}	6.65
30	4.53×10^{-3}	5.17
40	2.20×10^{-3}	9.44
50	5.76×10^{-4}	11.74

Table 2

4 Noncoercive Equilibrium Problems

4.1 Problem statement

We again consider our Hilbert space Y, and we now denote the corresponding dual space by Y', with norm $\|\cdot\|_{Y'}$. From the Riesz representation theorem we know that for all $f \in Y'$ there exists a $\rho_f \in Y$ such that $(\rho_f, v)_Y = f(v), \forall v \in Y$. It is then readily deduced that

$$\rho_f = \arg \sup_{v \in Y} \frac{f(v)}{\|v\|_Y},$$

and that $||f||_{Y'} = ||\rho_f||_Y$.

Our problem is then: given a parameter μ in the set $\mathcal{D} \subset \mathbb{R}^P$, and a linear functional $\ell \in Y'$, find $u(\mu) \in Y$ such that $a(u(\mu), v; \mu) = \ell(v), \forall v \in Y$, where $a(\cdot, \cdot; \mu)$ is a bilinear form the assumptions on which are detailed below. We further prescribe an output functional $\ell^O \in Y'$, in terms of which we can evaluate our output of interest $s(\mu) = \ell^O(u(\mu))$. The dual, or adjoint, problem associated with ℓ^O is defined as in Section 2.1.

We shall make the assumption that our bilinear form a is affine in the parameter μ as summarized by (3). We shall further assume (though this is not essential) that a is symmetric, $a(w,v;\mu)=a(v,w;\mu), \forall w,v\in Y^2, \forall \mu\in\mathcal{D}$. Finally, we assume that a is uniformly continuous, $|a(w,v;\mu)|\leq \gamma ||w||_Y||v||_Y, \forall w,v\in Y^2, \forall \mu\in\mathcal{D}$, and that a satisfies a uniform inf-sup condition: $\forall \mu\in\mathcal{D}$

$$(9) 0 < \beta_0 \le \beta(\mu) = \inf_{w \in Y} \sup_{v \in Y} \frac{a(w, v; \mu)}{\|w\|_Y \|v\|_Y} = \inf_{w \in Y} \frac{\|a(w, \cdot; \mu)\|_{Y'}}{\|w\|_Y} = \frac{\|a(\chi(\mu), \cdot; \mu)\|_{Y'}}{\|\chi(\mu)\|_Y}$$

where

$$\chi(\mu) = \arg \inf_{w \in Y} \frac{\|a(w, .; \mu)\|_{Y'}}{\|w\|_{Y}}.$$

It is classical that these final two conditions are required for well-posedness of our primal and dual problems.

4.2 Reduced-Basis Approximation

We first define the sample set $S_M = \{\mu_1, \dots, \mu_M\}$, and introduce three spaces $W_{M,u} = \text{span}\{u(\mu_i), i = 1, \dots, M\}$, $W_{M,\psi} = \text{span}\{\psi(\mu_i), i = 1, \dots, M\}$, and $W_{M,\chi} = \text{span}\{\chi(\mu_i), i = 1, \dots, M\}$, associated with our primal solutions, dual solutions, and infimizers, respectively. We then set N = 3M, and define our reduced-basis space W_N as

(10)
$$W_N = \text{span}\{u(\mu_1), \psi(\mu_1), \chi(\mu_1), \dots, u(\mu_M), \psi(\mu_M), \chi(\mu_M)\} \equiv \text{span}\{\zeta_1, \dots, \zeta_N\}.$$

Defining the primal and dual residual for the reduced-basis approximation as $R_N^{pr}(v; w^N; \mu) \equiv \ell(v) - a(w^N, v; \mu), \forall v \in Y$, and $R_N^{du}(v; \varphi^N; \mu) \equiv -\ell^O(v) - a(v, \varphi^N; \mu), \forall v \in Y$, respectively, we then look for $u_N(\mu) \in W_N, \psi_N(\mu) \in W_N$, $u_N(\mu) = \arg\inf_{w_N \in W_N} \|R_N^{du}(\cdot; w^N; \mu)\|_{Y'}$. Our output approximation is then given by $s_N(\mu) = \ell^O(u_N) - R_N^{pr}(\psi_N; u_N; \mu)$: The larger supremizing space is to ensure that the reduced-basis problem is well-posed and stable, thus yielding optimal convergence rates [6]. The additional adjoint terms improve the accuracy [10].

4.3 Error Estimation

We first define $\beta_N(\mu) \in \mathbb{R}$ as

(11)
$$\beta_N(\mu) = \inf_{w_N \in W_N} \sup_{v \in Y} \frac{a(w_N, v; \mu)}{\|w_N\|_Y \|v\|_Y} = \inf_{w_N \in W_N} \frac{\|a(w_N, \cdot; \mu)\|_{Y'}}{\|w_N\|_Y} = \frac{\|a(\chi_N(\mu), \cdot; \mu)\|_{Y'}}{\|\chi_N(\mu)\|_Y}$$

where

(12)
$$\chi_N(\mu) = \arg\inf_{w_N \in W_N} \frac{\|a(w_N, \cdot; \mu)\|_{Y'}}{\|w_N(\mu)\|_Y}$$

is our infimizer over W_N . The inclusion of the $\chi(\mu_i)$, $i=1,\ldots,M$, ensures the good approximation of β_N , and hence bounds [6].

Then, given $u_N(\mu), \psi_N(\mu)$, and a real constant α , $0 < \alpha < 1$, we compute

(13)
$$\Delta_N(\mu) \equiv \frac{1}{\alpha \beta_N(\mu)} \|R_N^{pr}(\cdot; u_N(\mu); \mu)\|_{Y'} \|R_N^{du}(\cdot; \psi_N(\mu); \mu)\|_{Y'},$$

and then $s_N^{\pm}(\mu) = s_N(\mu) \pm \Delta_N(\mu)$. The dual norms required in (13) are calculated by duality, just as in the coercive and eigenvalue formulations. It can then be shown [6], under certain assumptions, that s_N^{\pm} constitute asymptotic bounds for $s(\mu)$, and furthermore that the associated effectivities are bounded independent of N.

4.4 Blackbox formulation and Numerical Results

As for the earlier formulations, this noncoercive method also admits a two-stage off-line/on-line computational approach; and, as before, the computational complexity of the on-line stage scales only with N and Q. It is important to note [6] that it is the *same* precomputed influence functions that are required both to evaluate the residual norms in (13) and to develop the minimum residual approximation of Section 4.2: there is thus no penalty as regards either storage or computational complexity associated with our choice of larger supremizing space Y.

For numerical results of the method, as applied to the (noncoercive) Helmholtz problem, see [6]. In summary, increasing the dimension of the reduced-basis space yields very fast convergence of the bounds; furthermore, the effectivities are O(1). Bounds are obtained in all cases, except when there is an insufficient number of basis functions to accurately approximate the inf-sup parameter — exactly as suggested by the theory.

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