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"Natural norm" a posteriori error estimators for reduced basis approximations

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Abstract

We present a technique for the *rapid* and *reliable* prediction of linear-functional outputs of coercive and non-coercive linear elliptic partial differential equations with affine parameter dependence. The essential components are: (i) rapidly convergent global reduced basis approximations – (Galerkin) projection onto a space W_N spanned by solutions of the governing partial differential equation at N judiciously selected points in parameter space; (ii) a posteriori error estimation – relaxations of the error-residual equation that provide inexpensive yet sharp bounds for the error in the outputs of interest; and (iii) offline/online computational procedures – methods which decouple the generation and projection stages of the approximation process. The operation count for the online stage – in which, given a new parameter value, we calculate the output of interest and associated error bound – depends only on N (typically very small) and the parametric complexity of the problem.

In this paper we propose a new "natural norm" formulation for our reduced basis error estimation framework that: (a) greatly simplifies and improves our inf–sup lower bound construction (offline) and evaluation (online) – a critical ingredient of our a posteriori error estimators; and (b) much better controls – significantly sharpens – our output error bounds, in particular (through deflation) for parameter values corresponding to nearly singular solution behavior. We apply the method to two illustrative problems: a coercive Laplacian heat conduction problem – which becomes singular as the heat transfer coefficient tends to zero; and a non-coercive Helmholtz acoustics problem – which becomes singular as we approach resonance. In both cases, we observe very economical and sharp construction of the requisite natural-norm inf–sup lower bound; rapid convergence of the reduced basis approximation; reasonable effectivities (even for near-singular behavior) for our deflated output error estimators; and significant – several order of magnitude – (online) computational savings relative to standard finite element procedures.

Keywords: Parametrized partial differential equations; Reduced basis methods; Galerkin approximation; Inf–sup constant; Output bounds; A posteriori error estimation; Adjoint methods; Deflation

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1. Introduction

1.1. Reduced basis approach

Engineering analysis requires the prediction of an (or more realistically, several) "output of interest" $s^e \in \mathbb{R}$ – related to energies or forces, stresses or strains, flowrates or pressure drops, temperatures or fluxes – as a function of an "input" parameter P-vector $\mu \in \mathscr{D} \subset \mathbb{R}^P$ – related to geometry, physical properties, boundary conditions, or loads. These outputs $s^e(\mu)$ are often functionals of a field variable $u^e(\mu)$,

$$s^e(\mu) = \ell(u^e(\mu)), \tag{1}$$

where $u^e(\mu) \in X^e$ – say displacement, velocity, or temperature – satisfies in weak form the μ-parametrized (elliptic linear) partial differential equation

$$a(u^e(\mu), v; \mu) = f(v) \quad \forall v \in X^e. \tag{2}$$

Here X^e is the appropriate function space, and a (respectively ℓ, f) are continuous bilinear (respectively, linear) forms.

In general, we cannot find the exact (our superscript "e" above) solution, and hence we replace $s^e(\mu)$, $u^e(\mu)$ with a Galerkin finite element approximation, $s^{\mathscr{N}}(\mu), u^{\mathscr{N}}(\mu)$: given $\mu \in \mathscr{D}$,

$$s^{\mathscr{N}}(\mu) = \ell(u^{\mathscr{N}}(\mu)), \tag{3}$$

where $u^{\mathscr{N}}(\mu) \in X^{\mathscr{N}}$ satisfies

$$a(u^{\mathscr{N}}(\mu), v; \mu) = f(v) \quad \forall v \in X^{\mathscr{N}}. \tag{4}$$

Here $X^{\mathscr{N}} \subset X^e$ is a standard finite element approximation subspace of dimension $\mathscr{N}$. Unfortunately, to achieve the desired accuracy, $\mathscr{N}$ must typically be chosen very large; as a result, the evaluation $\mu \to s^{\mathscr{N}}(\mu)$ is simply too costly in the many-query and real-time contexts often of interest in engineering. Low-order models – we consider here reduced basis approximations – are thus increasingly popular in the engineering analysis, parameter estimation, design optimization, and control contexts.

In the reduced basis approach [1–7], we approximate $s^{\mathscr{N}}(\mu), u^{\mathscr{N}}(\mu)$ – for some fixed sufficiently large "truth" $\mathscr{N} = \mathscr{N}_t$ – with $s_N(\mu)$, $u_N(\mu)$: given $\mu \in \mathscr{D}$,

$$s_N(\mu) = \ell(u_N(\mu)), \tag{5}$$

where $u_N(\mu) \in W_N$ satisfies[1]

$$a(u_N(\mu), v; \mu) = f(v) \quad \forall v \in W_N. \tag{6}$$

Here W_N is a problem-specific space of dimension $N \ll \mathscr{N}_t$ that focuses on the (typically very smooth) parametric manifold of interest – $\{u^{\mathscr{N}_t}(\mu) | \mu \in \mathscr{D}\}$ – and thus enjoys very rapid convergence $u_N(\mu) \to u^{\mathscr{N}_t}(\mu)$ and hence $s_N(\mu) \to s^{\mathscr{N}_t}(\mu)$ as N increases [3,8]. This dramatic *dimension reduction*, in conjunction with *offline/online computational procedures* [6,7,9,10], yields very large savings in the many-query and real-time contexts: the online complexity depends only on the size of the reduced basis space, N, which is typically orders of magnitude smaller than the dimension of the finite element space, $\mathscr{N}_t$.

Our own effort is dedicated to the development of a posteriori error estimators for reduced basis approximations [6,7,11,12]: inexpensive – complexity *independent* of $\mathscr{N}_t$ – and sharp error bounds $\Delta_N^s(\mu)$ such that

$$|s^{\mathscr{N}_t}(\mu) - s_N(\mu)| \leqslant \Delta_N^s(\mu) \quad \forall \mu \in \mathscr{D}.$$

Absent such rigorous error bounds we cannot efficiently determine if N is too small – and our reduced basis approximation unacceptably inaccurate – or if N is too large – and our reduced basis approximation unnecessarily expensive. (Furthermore, in the nonlinear context, error bounds are crucial in establishing the very *existence* of a "truth" solution $u^{\mathscr{N}_t}(\mu)$ [13–15].) We cannot determine in "real-time" if critical design conditions and constraints are satisfied – for example, does approximate feasibility $s_N(\mu) \leqslant C$ imply "true" feasibility $s^{\mathscr{N}_t}(\mu) \leqslant C$? And, in fact, we can not even construct an efficient and well-conditioned reduced basis approximation space W_N [12,16].

[1] For simplicity in this Introduction, we consider a purely primal approach; we shall subsequently pursue a primal–dual formulation.

In this paper we focus on error estimators for (coercive and non-coercive) linear elliptic partial differential equations with affine parameter dependence. (For parabolic problems see [17]; for nonlinear problems, including the incompressible Navier–Stokes equations, see [11,12,14,15]; and for non-affine parameter dependence, see [16,18,19].) Relative to our earlier work, we introduce a new "natural norm" that (a) greatly simplifies and improves our inf–sup lower bound construction and evaluation – a critical ingredient of our error estimators [11,12,15]; and (b) much better controls the effectivity of – significantly sharpens – our error bounds, in particular (through deflation [11]) for nearly singular problems. We describe the formulation and provide several illustrative numerical examples.

1.2. Application to uncertainty quantification

In general, uncertainty quantification must account for (a) error introduced by the numerical discretization, (b) error or variance introduced by the input data, and (c) error introduced by the mathematical model. Our error estimators directly address (a) within the reduced basis approximation context. However, reduced basis error estimators are also an important "enabling technology" for the treatment of (b) and (c). Our emphasis in this paper is on the enabling technology per se – the reduced basis error estimators; however, we briefly consider here an application of our enabling technology to (b) and (c) – in particular, real-time parameter estimation – as an illustration of broader relevance to the themes of this Special Volume.

For our abstract inverse problem [20,21], we decompose $\mu \equiv (v, \sigma)$ and $\mathcal{D} = \mathcal{D}_v \times \mathcal{D}_\sigma$; here v represents the (say, P_v) parameters to be determined, and σ represents the ($P_\sigma = P - P_v$) parameters to be "controlled." We presume that we are given a set of experimental intervals I_j such that $s(v^*, \sigma_j) \in I_j$, $1 \leqslant j \leqslant J$, where $v^* \in \mathcal{D}_v$ is the value of the unknown parameter, and the $\sigma_j \in \mathcal{D}_\sigma, 1 \leqslant j \leqslant J$, are the specified values of the experimental control parameter. We then wish to determine – in the field, in real time – the "possibility" region $\mathcal{P} \equiv \{v \in \mathcal{D}_v | s(v, \sigma_j) \in I_j, 1 \leqslant j \leqslant J\}$ containing all values of v (including, of course, v^*) consistent with the experimental data: we wish to quantify the uncertainty in the unknown parameter. (More simply, we may find $v_m^{\min} \equiv \min_{v \in \mathcal{P}} v_m$ and $v_m^{\max} \equiv \max_{v \in \mathcal{P}} v_m, 1 \leqslant m \leqslant P_v$, from which we can construct the minimal box that contains $\mathcal{P}$, $\mathcal{B} = \prod_{m=1}^{P_v} [v_m^{\min}, v_m^{\max}]$.) Unfortunately, real-time construction of $\mathcal{P}$ (or $\mathcal{B}$) is typically not computationally viable.

We might thus consider the approximate reduced basis possibility region $\mathcal{P}_N^o \equiv \{v \in \mathcal{D}_v | s_N(v, \sigma_j) \in I_j, 1 \leqslant j \leqslant J\}$. However, $\mathcal{P}_N^o$ may not include v^*, in which case we risk an infeasible or unsafe decision (in, say, a subsequent robust optimization framework [22]); alternatively, $\mathcal{P}_N^o$ may be much larger than $\mathcal{P}$, in which case we risk an overly pessimistic decision. We should thus instead construct the approximate possibility region [16,18,22] $\mathcal{P}_N \equiv \{v \in \mathcal{D}_v | [s_N(v, \sigma_j) - \Delta_N^s(v, \sigma_j), s_N(v, \sigma_j) + \Delta_N^s(v, \sigma_j)] \cap I_j \neq \emptyset, 1 \leqslant j \leqslant J\}$. The certainty provided by our error bound simultaneously provides (i) efficiency, and hence rapid response: we may choose N (minimally) such that the reduced basis error $\Delta_N^s(\mu)$ is commensurate with the experimental error, and (ii) feasibility and safety: our approximate possibility region now *perforce includes the "true" possibility region*, $(v^* \in)\mathcal{P} \subset \mathcal{P}_N$. We refer the reader to [16,18,22] for applications of this reduced basis uncertainty quantification to non-destructive evaluation of cracks.

There are of course many alternative approaches to inverse problems and uncertainty quantification more generally, from Monte Carlo methods [23] to Bayesian techniques [24–26] to polynomial chaos expansions [27]. Our reduced basis enabling technology can readily serve in all these frameworks, providing for extremely accurate and rapid (and exhaustive) evaluation without – thanks to our error bounds – introducing a major new source of (numerical) uncertainty. (There are certainly other examples of the application of low-dimensional models to uncertainty quantification (e.g., [24]); however, rigorous a posteriori error control has received relatively little attention.)

2. Problem statement

2.1. Abstract formulation

Our exact output and field variable, $s^e(\mu) \in \mathbb{R}$ and $u^e(\mu) \in X^e$, satisfy (1), (2). Here, for any $\mu \equiv (\mu_1 \cdots \mu_P)$ in our closed input domain $\mathcal{D} \subset \mathbb{R}^P$, $a(\cdot, \cdot; \mu) : X^e \times X^e \to \mathbb{R}$ is a parameter-dependent bilinear form, and

$\ell : X^e \to \mathbb{R}$ and $f : X^e \to \mathbb{R}$ are parameter-independent linear forms (extension to parameter-dependent linear forms is straightforward). (See [16,28] for treatment of complex-valued fields with application to inverse scattering and acoustics more generally.) We shall consider second-order partial differential equations, and hence our exact space X^e satisfies $H_0^1(\Omega) \subset X^e \subset H^1(\Omega)$: here $\Omega \subset \mathbb{R}^d$ ($d = 1$, 2, or 3) is a spatial domain with suitably regular boundary $\partial\Omega$; and $H^1(\Omega)$ (respectively, $H_0^1(\Omega)$) is the usual Hilbert space of derivative-square-integrable functions (respectively, derivative-square-integrable functions that vanish on $\partial\Omega$).

Our "truth" or "reference" finite element approximation to the exact output and field variable, $s(\mu) \equiv s^{\mathcal{N}_t}(\mu)$ and $u(\mu) \equiv u^{\mathcal{N}_t}(\mu) \in X^{\mathcal{N}_t} \equiv X$, satisfies (3), (4) for the particular choice $\mathcal{N} = \mathcal{N}_t$. Given $\mu \in \mathcal{D}$,

$$s(\mu) = \ell(u(\mu)), \tag{7}$$

where $u(\mu) \in X$ satisfies

$$a(u(\mu), v; \mu) = f(v) \quad \forall v \in X. \tag{8}$$

We assume that $\mathcal{N}_t$ is chosen sufficiently large that $s(\mu)$ and $u(\mu)$ are essentially indistinguishable from $s^e(\mu)$ and $u^e(\mu)$, respectively. We shall build our reduced basis approximation upon this "truth" approximation; and we shall evaluate the error in our reduced basis approximation with respect to this "truth" approximation. As we will subsequently prove (see Section 7 and the Appendix), the online complexity (and stability) of our reduced basis approach is *independent* of $\mathcal{N}_t$; hence, we may choose $\mathcal{N}_t$ to be "arbitrarily" large at *no detriment to (online) performance*.

In addition to our "truth" primal problem, we shall also require a "truth" dual (or adjoint) problem [7,29–31] associated with our particular output functional. Given $\mu \in \mathcal{D}$,

$$s(\mu) = -f(\psi(\mu)), \tag{9}$$

where the adjoint $\psi(\mu) \in X$ satisfies

$$a(v, \psi(\mu); \mu) = -\ell(v) \quad \forall v \in X. \tag{10}$$

It follows from the primal problem (8) and the dual problem (10) that

$$\ell(u(\mu)) = -a(u(\mu), \psi(\mu); \mu) = -f(\psi(\mu)); \tag{11}$$

hence, (9) is a direct result of (10). Note that in the case of *compliance* – defined as (i) a symmetric: $a(w, v; \mu) = a(v, w; \mu)$ $\forall w, v \in X$, and (ii) $\ell = f$ – we obtain $\psi(\mu) = -u(\mu)$. We introduce the dual problem (10) and the adjoint variable $\psi(\mu)$ to improve the convergence of the output; we discuss this further in Section 4, in particular Lemma 4.1.

We shall suppose that our bilinear form is "affine" in the parameter: for some fixed integer Q – typically Q shall be larger than P, sometimes by a considerable factor – we require

$$a(w, v; \mu) = \sum_{q=1}^{Q} \Theta^q(\mu) a^q(w, v) \quad \forall w, v \in X, \ \forall \mu \in \mathcal{D}, \tag{12}$$

where $\Theta^q : \mathcal{D} \to \mathbb{R}$ and $a^q(w, v) : X \times X \to \mathbb{R}, 1 \leqslant q \leqslant Q$, are parameter-dependent functions and parameter-independent continuous bilinear forms, respectively. We shall further assume that $\Theta^q \in \mathcal{C}^1(\mathcal{D}), 1 \leqslant q \leqslant Q$. "Simple affine" (respectively, "general affine") shall refer to the case in which all the Θ^q, $1 \leqslant q \leqslant Q$, are affine functions of μ (respectively, at least one of the Θ^q, $1 \leqslant q \leqslant Q$, is not an affine function of μ).

We denote the inner product and norm associated with our Hilbert space $X(\equiv X^{\mathcal{N}_t})$ as $(w, v)_X$ and $\|v\|_X = \sqrt{(v, v)_X}$, respectively. We further define the dual norm for any bounded linear functional h as

$$\|h\|_{X'} \equiv \sup_{v \in X} \frac{h(v)}{\|v\|_X}; \tag{13}$$

recall that X is finite-dimensional. A typical choice for our inner product $(\cdot,\cdot)_X$ is

$$(w, v)_X = \int_\Omega \nabla w \cdot \nabla v + wv, \tag{14}$$

which is simply the standard $H^1(\Omega)$ inner product. Any inner product which induces a norm equivalent to the H^1 norm is acceptable.

We next introduce [11,12,22,29] the parametrized linear operator $T^\mu: X \to X$ such that, for any μ in $\mathcal{D}$ and any w in X,

$$(T^\mu w, v)_X = a(w, v; \mu) \quad \forall v \in X. \tag{15}$$

The classical inf–sup parameter and continuity parameter can then be expressed as

$$\beta(\mu) \equiv \inf_{w\in X} \sup_{v\in X} \frac{a(w, v; \mu)}{\|w\|_X \|v\|_X} \equiv \inf_{w\in X} \frac{\|T^\mu w\|_X}{\|w\|_X} \tag{16}$$

and

$$\gamma(\mu) \equiv \sup_{w\in X} \sup_{v\in X} \frac{a(w, v; \mu)}{\|w\|_X \|v\|_X} \equiv \sup_{w\in X} \frac{\|T^\mu w\|_X}{\|w\|_X}. \tag{17}$$

(Note that, from the Cauchy–Schwarz inequality, $v = T^\mu w$ is the inner supremizer in (16) and (17).)

We now suppose that $0 < \beta_0 \leqslant \beta(\mu) \leqslant \gamma(\mu) \leqslant \gamma_0 < \infty \ \forall \mu \in \mathcal{D}$ (note we may strengthen this requirement to hold for all $\mathcal{N} \geqslant \mathcal{N}_t$); we further assume that $\ell \in X'$ and $f \in X'$ – bounded linear functionals. It then follows that our primal and dual "truth" problems, (8) and (10), respectively, are well posed for all μ in $\mathcal{D}$.

Our method – in particular our inf–sup lower bound and our deflated adjoint approximation – requires a discrete set of K parameter values, $\mathcal{V}^K \equiv \{\overline{\mu}_1, \ldots, \overline{\mu}_K\} \subset \mathcal{D}$ – upon which to construct local corrections. It shall also prove convenient to introduce an indicator function $\mathcal{I}^K : \mathcal{D} \to \mathcal{V}^K$ which associates to any μ in $\mathcal{D}$ a member of $\mathcal{V}^K$. (The process by which we select "good" $\mathcal{V}^K$ and $\mathcal{I}^K$ is described in Section 5.)

We may then introduce, for given $\overline{\mu} \in \mathcal{V}^K$, our "natural inner product" and "natural norm" as

$$(((w, v)))_{\overline{\mu}} \equiv (T^{\overline{\mu}} w, T^{\overline{\mu}} v)_X \quad \forall w, v \in X \tag{18}$$

and

$$|||v|||_{\overline{\mu}} \equiv \sqrt{(((v, v)))_{\overline{\mu}}} \equiv \|T^{\overline{\mu}} v\|_X \quad \forall v \in X, \tag{19}$$

respectively. Note that, thanks to our assumptions on $\beta(\mu)$ and $\gamma(\mu)$, (19) does indeed define a norm (equivalent to $\|\cdot\|_X$). (See [32] for a very different approach to, and very different application of, "natural norms" for non-symmetric (coercive) operators.)

We can also define a symmetric positive-semidefinite eigenproblem related to the (square of the) singular values of our partial differential operator: for given $\overline{\mu} \in \mathcal{V}^K \subset \mathcal{D}$, $(\Phi_i(\overline{\mu}), \rho_i(\overline{\mu})) \in X \times \mathbb{R}$, $i = 1, \ldots, \mathcal{N}_t$, satisfies

$$(T^{\overline{\mu}} \Phi_i(\overline{\mu}), T^{\overline{\mu}} v)_X = \rho_i(\overline{\mu})(\Phi_i(\overline{\mu}), v)_X \quad \forall v \in X; \tag{20}$$

the eigenvalues are ordered such that $0 < \rho_1 \leqslant \rho_2 \leqslant \cdots \leqslant \rho_{\mathcal{N}_t}$. We normalize our eigenfunctions as $\|\Phi_i(\overline{\mu})\|_X = 1, i = 1, \ldots, \mathcal{N}_t$, and hence orthogonality reads

$$(T^{\overline{\mu}} \Phi_i(\overline{\mu}), T^{\overline{\mu}} \Phi_j(\overline{\mu}))_X = \rho_i(\overline{\mu})(\Phi_i(\overline{\mu}), \Phi_j(\overline{\mu}))_X = \rho_i(\overline{\mu})\delta_{ij}, \quad 1 \leqslant i, j \leqslant \mathcal{N}_t, \tag{21}$$

where δ_{ij} is the Kronecker-delta symbol. We may then identify

$$\beta(\overline{\mu}) = \sqrt{\rho_1(\overline{\mu})} \tag{22}$$

and

$$\gamma(\overline{\mu}) = \sqrt{\rho_{\mathcal{N}_t}(\overline{\mu})}, \tag{23}$$

where $\beta(\overline{\mu})$ and $\gamma(\overline{\mu})$ are the classical inf–sup and continuity parameters defined in (16), (17) for the choice $\mu = \overline{\mu}$. We also identify the second singular value,

$$\beta^+(\overline{\mu}) \equiv \sqrt{\rho_2(\overline{\mu})}. \tag{24}$$

Finally, we define[2]

$$\chi(\overline{\mu}) \equiv \Phi_1(\overline{\mu})/\beta(\overline{\mu}) \quad (|||\chi(\overline{\mu})|||_{\overline{\mu}} = 1): \tag{25}$$

the function $\chi(\overline{\mu})$ minimizes the inf–sup parameter – and hence represents the most unstable "mode"; $T^{\overline{\mu}}\chi(\overline{\mu})$ is the corresponding supremizer.

2.2. Reduced basis error estimation

We take advantage of the abstract formulation to summarize the central result of the reduced basis methods developed in this paper – the *certified* and *sharp* output error bounds for (nearly singular) linear elliptic parametrized PDEs. We also provide a roadmap for the remainder of the paper.

Given $\mu \in \mathcal{D}$, we define $u_N(\mu)$ and $\psi_N(\mu)$ as the reduced basis approximations to the "truth" primal and dual fields $u(\mu)$ and $\psi(\mu)$; we denote the corresponding primal and dual residuals as

$$\begin{aligned} r_N^{\mathrm{pr}}(v;\mu) &= f(v) - a(u_N(\mu), v; \mu) \quad \forall v \in X, \\ r_N^{\mathrm{du}}(v;\mu) &= -\ell(v) - a(v, \psi_N(\mu); \mu) \quad \forall v \in X, \end{aligned} \tag{26}$$

respectively. The adjoint $\psi_N(\mu)$ is "deflated" to ensure that the dual residual is orthogonal to the most "unstable" mode $\chi(\overline{\mu})$ (for $\overline{\mu} = \mathcal{I}^K\mu$):

$$r_N^{\mathrm{du}}(\chi(\overline{\mu});\mu) = 0. \tag{27}$$

Recall that $\mathcal{I}^K : \mathcal{D} \to \mathcal{V}^K$ is an indicator function that associates to each $\mu \in \mathcal{D}$ a "representative" (in fact, "nearby") member of the discrete parameter set $\mathcal{V}^K$.

We can then define our output error bound: for given $\mu \in \mathcal{D}$ and thus $\overline{\mu} = \mathcal{I}^K\mu \in \mathcal{V}^K$,

$$\Delta_N^s(\mu) \equiv \frac{1}{g_{\overline{\mu}}(\mu)\beta^+(\overline{\mu})} \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'} \|r_N^{\mathrm{du}}(\cdot;\mu)\|_{X'}. \tag{28}$$

Here $\|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'}$ and $\|r_N^{\mathrm{du}}(\cdot;\mu)\|_{X'}$ are the dual norms of the primal and dual residuals, respectively, and $g_{\overline{\mu}}(\mu)\beta^+(\overline{\mu})$ is "effectively" (though not rigorously) a lower bound for $\beta^+(\mu)$ – the *second* singular value, (24). (Strictly speaking, $g_{\overline{\mu}}(\mu)$ is a lower bound to an *order-unity* natural-norm inf–sup parameter defined in Section 5.) The form of (28) is in some sense standard: a residual divided by a stability factor.

We prove in Section 6 that

$$|s(\mu) - s_N(\mu)| \leqslant \Delta_N^s(\mu) \quad \forall \mu \in \mathcal{D}. \tag{29}$$

Deflation, (27), eliminates (an approximation to) the most unstable mode, which in turn eliminates $\beta(\mu)$ – the *first* singular value, (22) – in the error bound (28). Our result is particularly relevant for near-singular parameter values – parameter values for which $\beta(\mu) \equiv \sqrt{\rho_1(\mu)}$ is very small but (typically) $\beta^+(\mu) \equiv \sqrt{\rho_2(\mu)}$ remains "O(1)". (Note, however, that even for "regular" problems – for which $\beta(\mu) \approx \beta^+(\mu)$ – our procedure for the construction of the inf–sup lower bound function $g_{\overline{\mu}}(\mu)$ is still very useful.)

In Section 3, we introduce two illustrative instantiations to which we shall apply our reduced basis methodology. In Section 4, we describe the generation of the primal and dual reduced basis spaces and corresponding primal and deflated dual approximations, $u_N(\mu)$ and $\psi_N(\mu)$. In Section 5, we introduce our natural-norm inf–sup parameter and associated lower bound function, $g_{\overline{\mu}}(\mu)$. In Section 6, we describe our output error bound and prove the central result (29). Finally in Section 7, we briefly present a computational comparison of reduced basis methods (with error estimation) and standard finite element approaches for our two model problems; an Appendix presents the offline/online computational strategy by which we efficiently compute $s_N(\mu)$ and $\Delta_N^s(\mu)$.

[2] While the eigenproblem (20) and associated quantities (22)–(25) can be defined for any $\mu \in \mathcal{D}$, in practice we shall only need these entities for $\overline{\mu} \in \mathcal{V}^K \subset \mathcal{D}$.

3. Examples

3.1. Example I: Thermal plate fin – Laplacian

We consider a heat conduction problem corresponding to one unit of a thermal plate fin designed for the cooling of electronic components. We show in Fig. 1(a) the original domain of the problem $\Omega^o(L)$, consisting of a spreader subdomain of conductivity α (below) and a fin subdomain of conductivity unity and length L (above). The temperature field satisfies the Laplacian in the spreader–fin domain $\Omega^o(L)$. We impose unit heat flux (inhomogeneous Neumann) conditions on the spreader base Γ_B; periodic boundary conditions on the spreader vertical surfaces Γ_P; continuity of temperature and heat flux at the spreader–fin interface Γ_I; insulated (zero Neumann) conditions on the spreader and fin horizontal surfaces (shaded in Fig. 1); and a convection (Robin) boundary condition – with non-dimensional heat-transfer coefficient/Biot number Bi – on the fin vertical surfaces (exposed to the flowing air). We consider $P = 3$ parameters, $\mu_1 \equiv \alpha$, $\mu_2 \equiv (\mathrm{Bi}\, L)$, and $\mu_3 \equiv L$, for the parameter domain $\mathcal{D} = [1, 10] \times [0.025, 3.75] \times [2.5, 7.5]$.

In order to apply our methodology we map $\Omega^o(L) \rightarrow \Omega \equiv \Omega^o(L = L^{\mathrm{ref}} = 1)$, as shown in Fig. 1(b); the transformation is piecewise affine – the identity in the spreader/base, and a simple dilation in the fin. In these mapped coordinates, our bilinear form is given by

$$a(w, v; \mu) = \alpha \int_{\Omega_S} \nabla w \cdot \nabla v + (\mathrm{Bi}\, L) \int_{\Gamma_C} wv + L \int_{\Omega_F} \frac{\partial w}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{1}{L} \int_{\Omega_F} \frac{\partial w}{\partial x_2} \frac{\partial v}{\partial x_2}; \tag{30}$$

here $x = (x_1, x_2)$ is our mapped spatial coordinate, Ω_S and Ω_F are the mapped (and hence parameter-independent) spreader and fin subdomains, respectively, and Γ_C comprises the mapped vertical ("convection") surfaces of the fin. We observe that a is symmetric and coercive. Our linear form for the inhomogeneous Neumann condition is simply $f(v) \equiv \int_{\Gamma_B} v$, where we recall that Γ_B is the base of the spreader. Finally, $X^e \equiv H^1_{\#}(\Omega)$, in which # indicates periodicity on the vertical spreader surfaces Γ_P (except for periodicity, all other boundary conditions are natural); our truth approximation space $X = X^{\mathcal{N}_t}$ is a $\mathbb{P}_1$ (linear) finite element space of dimension $\mathcal{N}_t = 5300$.

We shall consider two outputs associated with two different output functionals. The first output $s_1(\mu)$ is the spreader base average temperature, corresponding to the output functional $\ell_1(v) \equiv f(v)$; since a is symmetric, this output functional is *compliant*. The output varies significantly with respect to all three parameters, from a minimum of 1.92 to a maximum of 23.58; there is a particularly steep increase as $\mathrm{Bi} \rightarrow 0$ – our problem is *singular* for $\mathrm{Bi} = 0$. The second output $s_2(\mu)$ is the average temperature at the spreader–fin interface, corresponding to the output functional $\ell_2(v) \equiv (1/0.3) \int_{\Gamma_I} v$; this output is of course *not* compliant. The second

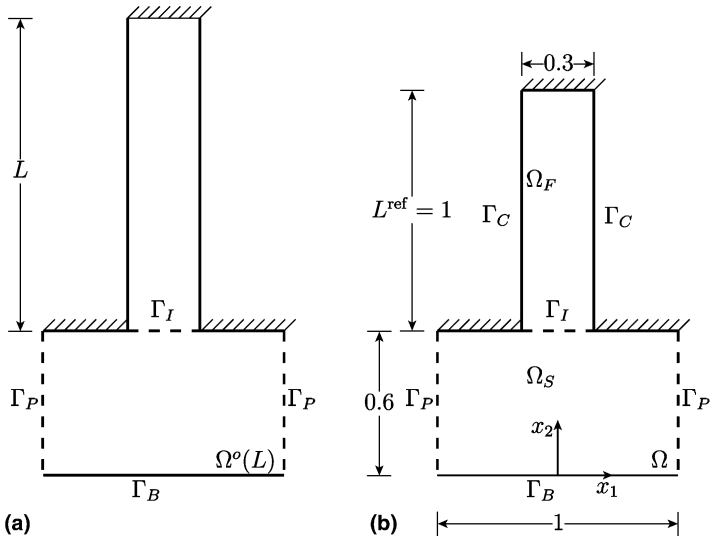

Fig. 1. Thermal plate fin: (a) original domain, and (b) reference/mapped domain.

output varies significantly with respect to ($\mathrm{Bi}\,L$) and L (but not with respect to α), from a minimum of 1.84 to a maximum of 22.71.

We observe that our bilinear form is indeed affine – "general affine" – as defined in (12). In particular, we identify $Q = 4$, with $\Theta^1(\mu) = \mu_1$, $\Theta^2(\mu) = \mu_2$, $\Theta^3(\mu) = \mu_3$, and $\Theta^4(\mu) = 1/\mu_3$. As will often be the case for "physical" parameters associated with material properties or geometric variations, a typical function $\Theta^q(\mu)$ will depend on only a few components of the parameter P-vector. (Obviously, the parametric representation is not unique, and hence we implicitly *choose* the $\Theta^q(\mu)$ with this "limited dependency" property.)

3.2. Example II: "Microphone probe" – Helmholtz

We consider a frequency-domain acoustics problem corresponding to a highly simplified microphone probe. We show in Fig. 2(a) the original domain of the problem $\Omega^o(L)$, consisting of an inlet (probe) and a cavity. The inlet in our non-dimensionalization is of length 1/2 and height 1/4; the cavity is of length 1 and height $(\frac{1}{4} + L)$. The pressure field satisfies the Helmholtz equation in $\Omega^o(L)$. We impose uniform unity pressure at the inlet Γ_{in}, Neumann symmetry conditions on the cavity centerline, and homogeneous Neumann (hence zero velocity) conditions on the walls. We shall consider $P = 2$ parameters, $\mu_1 \equiv k^2$ (the non-dimensional wavenumber squared), and $\mu_2 = L$, in the triangular parameter domain $\mathcal{D}$ shown in Fig. 3; we also plot in Fig. 3 the first resonance curve – for which this undamped system will be singular – which approaches quite closely to the parameter domain boundary.

In order to apply our methodology we map $\Omega^o(L) \rightarrow \Omega \equiv \Omega^o(L = L^{\text{ref}} = 1)$. As for the fin problem, the transformation is piecewise affine: the identity for the Lower part of the domain (inlet and cavity) – $\Omega_L \equiv]-\frac{1}{2}, 1[\times]0, \frac{1}{4}[$ for the mapped problem; and a simple dilation in the Upper part of the cavity – $\Omega_U \equiv]0, 1[\times]\frac{1}{4}, \frac{5}{4}[$ for the mapped problem. In these mapped coordinates, our bilinear form is given by

$$a(w, v; \mu) = \int_{\Omega_L} \nabla w \cdot \nabla v - k^2 \int_{\Omega_L} wv + L \int_{\Omega_U} \frac{\partial w}{\partial x_1} \frac{\partial v}{\partial x_1} + \frac{1}{L} \int_{\Omega_U} \frac{\partial w}{\partial x_2} \frac{\partial v}{\partial x_2} - k^2 L \int_{\Omega_U} wv, \tag{31}$$

where $x = (x_1, x_2)$ is the mapped coordinate. We observe that a is again symmetric (though our method is certainly not restricted to symmetric operators); however, a is no longer coercive. Our linear form $f(v; \mu)$ is given by $-a(U, v; \mu)$, where $U = -2x_1$ (respectively, 0) for $x_1 \leqslant 0$ (respectively, $x_1 > 0$); U is a lifting function for the inhomogeneous unity pressure boundary condition on Γ_{in}. Finally, $X^{\text{e}} = \{v \in H^1(\Omega) | v|_{\Gamma_{\text{in}}} = 0\}$ (except for the inflow pressure condition, all boundary conditions are natural); our truth approximation space $X = X^{\mathcal{N}_{\text{t}}}$ is a quadratic ($\mathbb{P}_2$) finite element space of dimension $\mathcal{N}_{\text{t}} = 4841$.

Finally, for our output, we consider a measure of the pressure over the right boundary of the cavity Γ_O – the "microphone surface" – corresponding to the output functional $\ell(v) = (1/(1/4 + L)) \int_{\Gamma_O} v$. (Note that our lifting function U vanishes for $x_1 > 0$ and hence on Γ_O; there is thus no contribution from U to the output.) This output varies significantly with respect to both parameters – from a minimum of close to unity (corresponding to faithful transducer performance) far from resonance to a maximum of 25 (corresponding to unwanted amplification) near the resonance/singular curve.

We observe that our bilinear form a is indeed affine – "general" affine – as defined in (12). In particular, we identify $Q = 5$, with $\Theta^1(\mu) = 1$, $\Theta^2(\mu) = -\mu_1 \equiv -k^2$, $\Theta^3(\mu) = \mu_2 \equiv L$, $\Theta^4(\mu) = 1/\mu_2 \equiv 1/L$, and $\Theta^5(\mu) = -\mu_1\mu_2 \equiv -k^2 L$. Note for this particular problem, our linear functional f and our output functional ℓ also depend

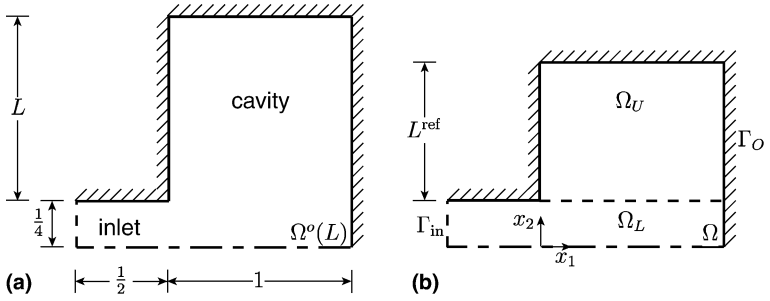

Fig. 2. "Microphone probe": (a) original domain, and (b) reference/mapped domain.

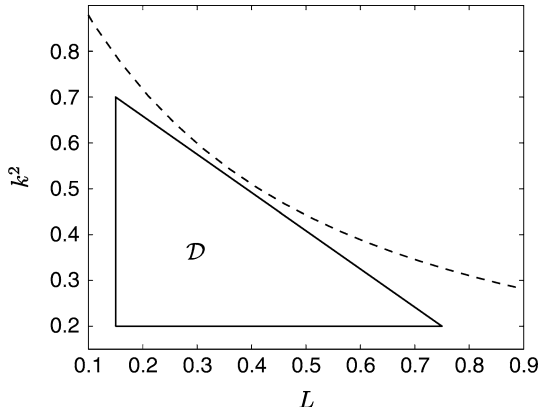

Fig. 3. Parameter domain $\mathscr{D}$ for the Helmholtz problem. The dashed line indicates the (first) resonance curve.

affinely on the parameter. For simplicity of presentation in this paper, we shall restrict our exposition of the methodology to the abstract formulation of Section 2, in which f and ℓ are independent of μ; the extension to affine parameter dependence of f and ℓ – reflected in the *results* for Example II – is very simple.

4. Reduced basis approximation

4.1. Formulation

We first define (in fact, relative to the Introduction, *re*define) $N = (N_{\rm pr}, N_{\rm du})$, where $N_{\rm pr}$ and $N_{\rm du}$ refer to the dimension of the primal and dual reduced basis approximation spaces. We also specify $N_{\rm pr,max}$ and $N_{\rm du,max}$ as the upper limits on the dimensions of the primal and dual spaces, respectively, which will determine the maximum reduced basis accuracy that can be achieved.

We next introduce sets of primal and dual parameter points, $\mu_n^{\rm pr},\ 1 \leqslant n \leqslant N_{\rm pr,max}$, and $\mu_n^{\rm du},\ 1 \leqslant n \leqslant N_{\rm du,max}$, respectively. Our primal (Lagrangian [4]) reduced basis nested approximation spaces are then given by $W_{N_{\rm pr}}^{\rm pr} \equiv {\rm span}\{u(\mu_n^{\rm pr}), 1 \leqslant n \leqslant N_{\rm pr}\}, 1 \leqslant N_{\rm pr} \leqslant N_{\rm pr,max}$, where the $u(\mu_n^{\rm pr}), 1 \leqslant n \leqslant N_{\rm pr,max}$, are our "snapshots." We express (any member of) $W_{N_{\rm pr}}^{\rm pr}$ in terms of the basis $\zeta_n^{\rm pr}, 1 \leqslant n \leqslant N_{\rm pr}$, where the $\zeta_n^{\rm pr}, 1 \leqslant n \leqslant N_{\rm pr,max}$, are generated from the $u(\mu_n^{\rm pr}), 1 \leqslant n \leqslant N_{\rm pr,max}$, by a Gram–Schmidt orthogonalization process relative to the $(\cdot,\cdot)_X$ inner product. In an analogous fashion, we create our dual reduced basis nested approximation spaces as $W_{N_{\rm du}}^{\rm du} \equiv {\rm span}\{\psi(\mu_n^{\rm du}), 1 \leqslant n \leqslant N_{\rm du}\} \equiv {\rm span}\{\zeta_n^{\rm du}, 1 \leqslant n \leqslant N_{\rm du}\}, 1 \leqslant N_{\rm du} \leqslant N_{\rm du,max}$.[3]

Then, for given $\mu \in \mathscr{D}$, our primal approximation $u_N(\mu) \in W_{N_{\rm pr}}^{\rm pr}$ satisfies

$$a(u_N(\mu), v; \mu) = f(v) \quad \forall v \in W_{N_{\rm pr}}^{\rm pr}; \tag{32}$$

we denote the primal residual as

$$r_N^{\rm pr}(v; \mu) \equiv f(v) - a(u_N(\mu), v; \mu) \quad \forall v \in X, \tag{33}$$

and the primal error as

$$e^{\rm pr}(\mu) \equiv u(\mu) - u_N(\mu). \tag{34}$$

We presume that (32) is well-posed and yields a unique solution. (Although Petrov–Galerkin approaches may be preferable for (provable) discrete stability [29], in actual practice Galerkin reduced basis methods typically suffice even for non-coercive problems.)

[3] In actual practice, our primal and dual sample points and associated primal and dual approximation spaces are constructed by a greedy selection process – based on the a posteriori error estimation procedures of the next section – that ensures "maximally independent" snapshots (in parameter space) and hence a rapidly convergent reduced basis approximation. In conjunction with our orthogonalization procedure, this sampling strategy also guarantees a well-conditioned reduced basis discrete system [16]. Details of this sampling procedure may be found in [11,12] for elliptic problems and [17,18] for parabolic problems.

Our "undeflated" dual approximation $\psi_N^o(\mu) \in W_{N_{\rm du}}^{\rm du}$ satisfies

$$a(v, \psi_N^o(\mu); \mu) = -\ell(v) \quad \forall v \in W_{N_{\rm du}}^{\rm du}; \tag{35}$$

we denote the associated "undeflated" residual and error as

$$r_N^{{\rm du},o}(v;\mu) \equiv -\ell(v) - a(v, \psi_N^o(\mu); \mu) \quad \forall v \in X, \tag{36}$$

and

$$e^{{\rm du},o}(\mu) \equiv \psi(\mu) - \psi_N^o(\mu), \tag{37}$$

respectively. We presume that (35) is well-posed and yields a unique solution.

For a given $\mu \in \mathscr{D}$ and associated $\overline{\mu} = \mathscr{I}^K \mu \in \mathscr{V}^K$, the deflated dual [11] approximation is then given by

$$\psi_N^{\mathscr{V}^K,\mathscr{I}^K}(\mu) = \psi_N^o(\mu) + \delta_{\overline{\mu}}(\mu), \tag{38}$$

where

$$\delta_{\overline{\mu}}(\mu) \equiv c_{\overline{\mu}}(\mu) T^{\overline{\mu}} \chi(\overline{\mu}) \tag{39}$$

satisfies

$$a(\chi(\overline{\mu}), \delta_{\overline{\mu}}(\mu); \mu) = r_N^{{\rm du},o}(\chi(\overline{\mu}); \mu). \tag{40}$$

We shall henceforth abbreviate $\psi_N^{\mathscr{V}^K,\mathscr{I}^K}$ as ψ_N; the dependence (through the deflation correction) on $\mathscr{V}^K$, $\mathscr{I}^K$ is understood. We denote the associated "deflated" residual and error as

$$r_N^{\rm du}(v;\mu) \equiv -\ell(v) - a(v, \psi_N(\mu); \mu) \quad \forall v \in X, \tag{41}$$

and

$$e^{\rm du}(\mu) \equiv \psi(\mu) - \psi_N(\mu), \tag{42}$$

respectively. We adopt the convention that $N_{\rm du} = 0$ corresponds to $\psi^o(\mu) = 0$; in this case, $\psi_N(\mu) = \delta_{\overline{\mu}}(\mu)$.

It can be shown that (40) is stable: under suitable (verifiable) hypotheses on $\mathscr{V}^K$, $\mathscr{I}^K$, we can directly relate $\|\delta_{\overline{\mu}}(\mu)\|_X$ to $\|e^{{\rm du},o}(\mu)\|_X$ – see Proposition 5.3 of Section 5 for the proof. Hence our deflation correction will not incommensurately adversely affect the dual error; indeed, deflation may reduce the dual error, though this is not guaranteed. The main purpose of deflation is to eliminate the component of the error – associated with the most unstable mode – that forces us, through our inf–sup lower bound, to treat in our error bound all error modes overly pessimistically (see Section 2.2). We discuss this in detail in the Section 6.

Finally, we shall define (in fact, relative to the Introduction, *re*define) our deflated reduced basis output approximation $s_N(\mu)$ as

$$s_N(\mu) \equiv \ell(u_N(\mu)) - r_N^{\rm pr}(\psi_N(\mu); \mu). \tag{43}$$

We can then prove

Lemma 4.1. *Under our assumption that the discrete problems (32), (35), and (40) are well posed, $s_N(\mu)$ of (43) satisfies*

$$s(\mu) - s_N(\mu) = -a(e^{\rm pr}(\mu), e^{\rm du}(\mu); \mu) = -r_N^{\rm du}(e^{\rm pr}(\mu); \mu) \quad \forall \mu \in \mathscr{D}. \tag{44}$$

Proof. We first note that $s(\mu) - s_N(\mu) = \ell(e^{\rm pr}(\mu)) + r_N^{\rm pr}(\psi_N(\mu); \mu)$, which, from the definition of our dual problem (10), can be expressed as $s(\mu) - s_N(\mu) = -a(e^{\rm pr}(\mu), \psi(\mu); \mu) + r_N^{\rm pr}(\psi_N(\mu); \mu)$. The result then directly follows from the standard primal and dual error-residual relationships, $r_N^{\rm pr}(v;\mu) = a(e^{\rm pr}(\mu), v; \mu)$ and $r_N^{\rm du}(v;\mu) = a(v, e^{\rm du}(\mu); \mu)$, respectively. □

We thus observe the usual "quadratic" convergence of the output relative to the primal and dual errors.

Remark 1. In the case of compliance – (i) a symmetric, and (ii) $\ell = f$ – we may replace (43) with

$$s_N(\mu) \equiv -\ell(\psi_N(\mu)) + r_N^{\rm du}(\psi_N(\mu); \mu) \quad \text{(compliance)} \tag{45}$$

and (44) of Lemma 4.1 with

$$s(\mu) - s_N(\mu) = a(e^{\mathrm{du}}(\mu), e^{\mathrm{du}}(\mu); \mu) = r_N^{\mathrm{du}}(e^{\mathrm{du}}(\mu); \mu) \quad \text{(compliance)}; \tag{46}$$

we no longer need the primal solution. (Of course, we can also rephrase the result solely in terms of a deflated primal; however, since our dual is already deflated, (46) is notationally more convenient.)

4.2. Numerical results

We present in Table 1 the convergence of the two outputs $s_1(\mu)$ and $s_2(\mu)$ – associated with output functionals $\ell_1(\mu)$ and $\ell_2(\mu)$, respectively – of Example I of Section 3.1, the thermal plate fin. We present the results in terms of N_{du}; for the first (compliant) output, there is no need for a primal solution – we invoke (45); for the second (non-compliant) output, we take $N_{\mathrm{pr}} = N_{\mathrm{du}}$. The error $E_{i,N}$ reported for each output, subscript $i = 1, 2$, is the maximum of the relative error, $|s_i(\mu) - s_{i,N}(\mu)|/|s_i(\mu)|$, over a random parameter test sample $\Xi_{\mathrm{test}}^{\mathrm{I}} \subset \mathcal{D}$ of size $n_{\mathrm{test}}^{\mathrm{I}} = 1000$. We observe very rapid convergence with N, as expected from the "smooth parametric manifold" arguments [3,8,12].

We present in Table 2 the convergence of the output associated with Example II of Section 3.2, the "microphone probe." We present the results in terms of N_{du} ($=N_{\mathrm{pr}}$). The error E_N is the maximum of the relative error, $|s(\mu) - s_N(\mu)|/|s(\mu)|$, over a random parameter test sample $\Xi_{\mathrm{test}}^{\mathrm{II}} \subset \mathcal{D}$ of size $n_{\mathrm{test}}^{\mathrm{II}} = 400$. As for the thermal fin, we observe very rapid convergence with N. Note that our parameter domain $\mathcal{D}$ – see Fig. 3 – only significantly excites a single (near-) resonant mode. If $\mathcal{D}$ were to approach other resonant modes (or, in the case of a damped system, to *include* other resonant modes), the reduced basis spaces would need to be suitably enlarged [11]. In general for Helmholtz problems – due to both approximation and certainly inf–sup lower bound considerations – we can only hope to address some modest number of resonances within any particular certified reduced basis approximation.

5. Inf–sup parameter: lower bound

Our error bound (28) requires an inexpensive (online) and reasonably accurate lower bound for a piecewise "natural-norm" inf–sup stability parameter. We first define the latter, and then construct the former – the function $g_{\overline{\mu}}(\mu)$ of Section 2.2.

Table 1
Example I, Thermal plate fin: the (maximum) relative error $E_{i,N}$, (maximum) a posteriori output error bound $\mathscr{E}_{i,N}$, and (average) effectivity $\overline{\eta}_{i,N}^{s}$, as a function of N_{du} for outputs s_1 and s_2

N_{du}	$E_{1,N}$	$\mathscr{E}_{1,N}$	$\overline{\eta}_{1,N}^{s}$	$E_{2,N}$	$\mathscr{E}_{2,N}$	$\overline{\eta}_{2,N}^{s}$
4	2.32E−02	8.28E−01	16.83	0.94E−02	4.85E−01	70.18
8	1.04E−03	2.25E−02	18.32	1.20E−04	5.13E−03	155.35
12	1.74E−05	7.29E−05	11.36	1.91E−06	4.61E−05	75.38
16	9.56E−07	9.73E−06	14.50	6.42E−07	6.63E−06	62.36
20	–	–	–	3.4E−08	7.12E−07	15.29

(See Section 6.2 for a discussion of the error bound and effectivity.)

Table 2
Example II, "Microphone probe": the (maximum) relative error E_N, (maximum) a posteriori output error bound $\mathscr{E}_N$, and (average) effectivity $\overline{\eta}_N^{s}$, as a function of N_{du}

N_{du}	E_N	$\mathscr{E}_N$	$\overline{\eta}_N^{s}$
2	8.56E−02	2.27E+00	35.58
4	3.72E−04	4.58E−03	52.17
6	1.52E−05	1.11E−04	33.33
8	4.34E−07	8.33E−06	40.05
10	9.00E−09	2.57E−07	15.14

(See Section 6.2 for a discussion of the error bound and effectivity.)

5.1. Natural-norm inf–sup parameter

To begin, for given $\mu \in \mathscr{D}$ and $\overline{\mu} \in \mathscr{V}^K$, we define local natural-norm inf–sup and continuity parameters as

$$\tilde{\beta}_{\overline{\mu}}(\mu) \equiv \inf_{w\in X} \sup_{v\in X} \frac{a(w,v;\mu)}{|||w|||_{\overline{\mu}}\|v\|_X} \equiv \inf_{w\in X} \frac{\|T^{\mu}w\|_X}{\|T^{\overline{\mu}}w\|_X} \tag{47}$$

and

$$\tilde{\gamma}_{\overline{\mu}}(\mu) \equiv \sup_{w\in X} \sup_{v\in X} \frac{a(w,v;\mu)}{|||w|||_{\overline{\mu}}\|v\|_X} \equiv \sup_{w\in X} \frac{\|T^{\mu}w\|_X}{\|T^{\overline{\mu}}w\|_X}, \tag{48}$$

respectively. It is clear that, for $\mu = \overline{\mu}$, $\tilde{\beta}_{\overline{\mu}}(\overline{\mu}) = \tilde{\gamma}_{\overline{\mu}}(\overline{\mu}) = 1$; our natural norm can thus be viewed as a generalization of the usual energy norm (for symmetric, coercive operators) to the non-symmetric non-coercive case. (Note the natural norms proposed in [32] for non-symmetric coercive operators, though very different in formulation, details, and application, are also characterized by order-unity inf–sup and continuity constants: this is arguably the essential property of any natural norm proposal.) It can be demonstrated that

$$\beta(\overline{\mu})\tilde{\beta}_{\overline{\mu}}(\mu) \leqslant \beta(\mu) \leqslant \tilde{\beta}_{\overline{\mu}}(\mu)\gamma(\overline{\mu}); \tag{49}$$

hence (under our assumptions on $\beta(\mu)$ and $\gamma(\mu)$), $\tilde{\beta}_{\overline{\mu}}(\mu)$ is bounded away from zero for all μ in $\mathscr{D}$.

In what follows we shall also require an "intermediate" inf–sup parameter – an approximation to $\tilde{\beta}_{\overline{\mu}}(\mu)$ – which we shall denote as $\overline{\beta}_{\overline{\mu}}(\mu)$: for given $\mu \in \mathscr{D}$ and $\overline{\mu} \in \mathscr{V}^K$,

$$\overline{\beta}_{\overline{\mu}}(\mu) \equiv \inf_{w\in X} \frac{(T^{\mu}w, T^{\overline{\mu}}w)_X}{|||w|||^2_{\overline{\mu}}}. \tag{50}$$

It follows directly from the Cauchy–Schwarz inequality – or equivalently, we may observe that $T^{\overline{\mu}}w$ is a candidate supremizer v in (47) – that $\overline{\beta}_{\overline{\mu}}(\mu)$ is a lower bound for $\tilde{\beta}_{\overline{\mu}}(\mu)$,

$$\overline{\beta}_{\overline{\mu}}(\mu) \leqslant \tilde{\beta}_{\overline{\mu}}(\mu) \quad \forall \mu \in \mathscr{D} \tag{51}$$

(note that $\overline{\beta}_{\overline{\mu}}(\mu)$ is not necessarily positive).

We can also show that $\overline{\beta}_{\overline{\mu}}(\mu)$ is a "good" lower bound for $\tilde{\beta}_{\overline{\mu}}(\mu)$; we sketch here the proof. We first expand $\tilde{\beta}^2_{\overline{\mu}}(\mu)$ to obtain

$$\begin{aligned}\tilde{\beta}^2_{\overline{\mu}}(\mu) &= \inf_{w\in X} \frac{\left(T^{\overline{\mu}}w + (T^{\mu}w - T^{\overline{\mu}}w), T^{\overline{\mu}}w + (T^{\mu}w - T^{\overline{\mu}}w)\right)_X}{\|T^{\overline{\mu}}w\|^2_X} \\ &= 1 + 2\inf_{w\in X} \frac{(T^{\mu}w - T^{\overline{\mu}}w, T^{\overline{\mu}}w)_X}{\|T^{\overline{\mu}}w\|^2_X} + \mathrm{O}(|\mu-\overline{\mu}|^2) = -1 + 2\overline{\beta}_{\overline{\mu}}(\mu) + \mathrm{O}(|\mu-\overline{\mu}|^2) \quad \text{as } \mu \to \overline{\mu}\end{aligned} \tag{52}$$

from the affine nature of a and our assumption $\Theta^q \in \mathscr{C}^1(\mathscr{D})$ (see the discussion following (12)); it thus follows that

$$\tilde{\beta}_{\overline{\mu}}(\mu) = \overline{\beta}_{\overline{\mu}}(\mu) + \mathrm{O}(\overline{\beta}_{\overline{\mu}}(\mu) - 1)^2 + \mathrm{O}(|\mu-\overline{\mu}|^2) \quad \text{as } \mu \to \overline{\mu}. \tag{53}$$

Finally, we again exploit the continuity of a to note that

$$\overline{\beta}_{\overline{\mu}}(\mu) - 1 = \mathrm{O}(|\mu-\overline{\mu}|) \quad \text{as } \mu \to \overline{\mu}; \tag{54}$$

therefore, $|\tilde{\beta}_{\overline{\mu}}(\mu) - \overline{\beta}_{\overline{\mu}}(\mu)| = \mathrm{O}(|\mu-\overline{\mu}|^2)$ as $\mu \to \overline{\mu}$, where $|\cdot|$ refers to the usual Euclidean norm. We conclude that $\overline{\beta}_{\overline{\mu}}(\mu)$ is a second-order accurate approximation to $\tilde{\beta}_{\overline{\mu}}(\mu)$ for μ near $\overline{\mu}$.

Finally, we recall our parameter set $\mathscr{V}^K \equiv \{\overline{\mu}_1 \in \mathscr{D}, \overline{\mu}_2 \in \mathscr{D}, \ldots, \overline{\mu}_K \in \mathscr{D}\}$ and associated "indicator" function $\mathscr{I}^K : \mathscr{D} \to \mathscr{V}^K$; $\mathscr{I}^K$ maps any given $\mu \in \mathscr{D}$ to a "representative" (in fact, "nearby") member of $\mathscr{V}^K$. Our global natural-norm inf–sup parameter is then assembled as

$$\tilde{\beta}^{\mathscr{V}^K,\mathscr{I}^K}(\mu) \equiv \inf_{w\in X} \sup_{v\in X} \frac{a(w,v;\mu)}{|||w|||_{\mathscr{I}^K\mu}\|v\|} = \tilde{\beta}_{\mathscr{I}^K\mu}(\mu); \tag{55}$$

we further define $\tilde{\beta}_{\min}^{\mathscr{V}^K,\mathscr{I}^K} \equiv \min_{\mu\in\mathscr{D}} \tilde{\beta}^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$. (Where there is no opportunity for confusion, we shall abbreviate $\tilde{\beta}^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$ as $\tilde{\beta}^K(\mu)$.) Note that as K increases and $\mathscr{V}^K$ becomes denser in $\mathscr{D}$, $\tilde{\beta}^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$ approaches unity for all $\mu \in \mathscr{D}$; the piecewise natural-norm inf–sup parameter is thus intrinsically "easy" to approximate. We now turn to the construction of a lower bound approximation.

5.2. Lower bound construction

5.2.1. Local lower bound

We begin with a local lower bound. Furthermore, for pedagogical purposes, we first consider the "simple affine" case; more precisely, we assume that $a(w, v; \mu)$ has the "simplest affine" form ($Q = P$)

$$a(w, v; \mu) = \sum_{p=1}^{P} \mu_p a^p(w, v),$$

where μ_p is the pth component of $\mu \in \mathbb{R}^P$ and the a^p, $1 \leqslant p \leqslant P$, are continuous bilinear forms.

Under this assumption, it follows from (50) and (15) that, for given $\mu \in \mathscr{D}$ and $\overline{\mu} \in \mathscr{V}^K$,

$$\overline{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu) = \inf_{w\in X} \frac{(T^{\overline{\mu}}w + (T^{\mu}w - T^{\overline{\mu}}w), T^{\overline{\mu}}w)_X}{|||w|||_{\overline{\mu}}^2} = 1 + \inf_{w\in X} \sum_{p=1}^{P} (\mu_p - \overline{\mu}_p) \frac{a^p(w, T^{\overline{\mu}}w)_X}{|||w|||_{\overline{\mu}}^2}$$

(here "sa" refers to "simplest affine"). Hence, if we introduce the extreme eigenvalues

$$\lambda_{\overline{\mu},\min}^{p,\mathrm{sa}} = \min_{w\in X} \frac{a^p(w, T^{\overline{\mu}}w)_X}{|||w|||_{\overline{\mu}}^2},$$

$$\lambda_{\overline{\mu},\max}^{p,\mathrm{sa}} = \max_{w\in X} \frac{a^p(w, T^{\overline{\mu}}w)_X}{|||w|||_{\overline{\mu}}^2},$$

then

$$g_{\overline{\mu}}^{\mathrm{sa}}(\mu) \equiv 1 + \sum_{p=1}^{P} \mathrm{Min}\left[(\mu_p - \overline{\mu}_p)\lambda_{\overline{\mu},\min}^{p,\mathrm{sa}}, (\mu_p - \overline{\mu}_p)\lambda_{\overline{\mu},\max}^{p,\mathrm{sa}}\right] = 1 + \sum_{p=1}^{P} \inf_{w\in X} \left((\mu_p - \overline{\mu}_p)\frac{a^p(w, T^{\overline{\mu}}w)_X}{|||w|||_{\overline{\mu}}^2}\right) \leqslant \overline{\beta}_{\overline{\mu}}(\mu).$$

Note $\mathrm{Min}[x, y]$ returns x if $x \leqslant y$ and y otherwise.

Thus $g_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ is a lower bound for $\overline{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ and, from (51), for $\tilde{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ as well. We also expect that $g_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ will be a reasonably good lower bound at least for μ near $\overline{\mu}$. In particular, we note from our derivation that $g_{\overline{\mu}}^{\mathrm{sa}}(\mu) = \overline{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ (exactly) along parameter coordinate directions – for any $\mu = \overline{\mu} + z$ for which $z \in \mathbb{R}^P$ is non-zero in only a single component. (Unfortunately, and despite (53), (54), the discrepancy $|\tilde{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu) - g_{\overline{\mu}}^{\mathrm{sa}}(\mu)|$ is not *generally* $\mathrm{O}(|\mu - \overline{\mu}|^2)$ even for μ near $\overline{\mu}$, since $\overline{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ and $\tilde{\beta}_{\overline{\mu}}^{\mathrm{sa}}(\mu)$ are not $\mathscr{C}^1(\mathscr{D})$.)

We now address the general affine case, (12), by an (almost) direct Taylor-series extension of the simplest affine case described above. To wit, for given $\mu \in \mathscr{D}$ and $\overline{\mu} \in \mathscr{V}^K$, we write

$$g_{\overline{\mu}}(\mu) = \max_{\kappa\in\mathbb{R}^P} \hat{g}_{\overline{\mu}}(\mu; \kappa), \tag{56}$$

where for given $\mu \in \mathscr{D}$ and $\overline{\mu} \in \mathscr{V}^K$,

$$\begin{aligned}\hat{g}_{\overline{\mu}}(\mu; \kappa) = 1 &+ \sum_{p=1}^{P} \mathrm{Min}\left[\kappa_p(\mu_p - \overline{\mu}_p)\lambda_{\overline{\mu},\max}^{p}, \kappa_p(\mu_p - \overline{\mu}_p)\lambda_{\overline{\mu},\min}^{p}\right] \\ &+ \sum_{q=1}^{Q}, \mathrm{Min}\left[\left(\Theta^q(\mu) - \Theta^q(\overline{\mu}) - \sum_{p'=1}^{P} \frac{\partial\Theta^q}{\partial\mu_{p'}}(\overline{\mu})\kappa_{p'}(\mu_{p'} - \overline{\mu}_{p'})\right)\xi_{\overline{\mu},\max}^{q},\right. \\ &\left.\left(\Theta^q(\mu) - \Theta^q(\overline{\mu}) - \sum_{p'=1}^{P} \frac{\partial\Theta^q}{\partial\mu_{p'}}(\overline{\mu})\kappa_{p'}(\mu_{p'} - \overline{\mu}_{p'})\right)\xi_{\overline{\mu},\min}^{q}\right];\end{aligned} \tag{57}$$

here, for $p = 1, \ldots, P$, $\lambda^p_{\overline{\mu},\min}$ and $\lambda^p_{\overline{\mu},\max}$ are given by

$$\lambda^p_{\overline{\mu},\min(\max)} = \min_{w\in X}(\max_{w\in X}) \frac{\sum_{q=1}^{Q} \frac{\partial \Theta^q}{\partial \mu_p}(\overline{\mu}) a^q(w, T^{\overline{\mu}} w)}{|||w|||^2_{\overline{\mu}}}, \tag{58}$$

and, for $q = 1, \ldots, Q$, $\xi^q_{\overline{\mu},\min}$ and $\xi^q_{\overline{\mu},\max}$ are given by

$$\xi^q_{\overline{\mu},\min(\max)} = \min_{w\in X}(\max_{w\in X}) \frac{a^q(w, T^{\overline{\mu}} w)}{|||w|||^2_{\overline{\mu}}}. \tag{59}$$

(In (58) and (59), min(max) refers to two different quantities.) Recall that the Min$[x, y]$ function returns x if $x \leqslant y$ and y otherwise.

We recognize the first two terms of (57), and the extreme eigenvalues (58), as the first-order Taylor series generalization of the "simplest affine" result; we recognize the third sum in (57), and the extreme eigenvalues (59), as the "remainder" term – which is of course absent in the simple affine case (for the choice $\kappa = 1$). The tuning parameter $\kappa \in \mathbb{R}^P$ in (57) is effectively a local rescaling of the parameter – there is implicitly much freedom in the parametric representation (see also Remark 3 below) – that is optimized in (56) to balance the various contributions to the lower bound. We shall denote the optimal scaling parameter as $\kappa^{\text{opt}}_{\overline{\mu}}(\mu) \equiv \arg\max_{\kappa\in\mathbb{R}^P} \hat{g}_{\overline{\mu}}(\mu; \kappa)$.

Remark 2. We note that, for *fixed* μ and $\overline{\mu}$, the optimization with respect to κ, (56), takes the form

$$g_{\overline{\mu}}(\mu) = 1 + \max_{\kappa\in\mathbb{R}^P} \sum_{m=1}^{P+Q} \text{Min}[F_m(\kappa), G_m(\kappa)], \tag{60}$$

where the F_m, G_m, $1 \leqslant m \leqslant P + Q$, are affine functions of κ. We may thus rewrite (60) as

$$g_{\overline{\mu}}(\mu) = 1 + \max_{\substack{\kappa\in\mathbb{R}^P, d\in\mathbb{R}^{P+Q} \\ F_m(\kappa)\geqslant d_m, G_m(\kappa)\geqslant d_m, 1\leqslant m\leqslant P+Q}} \sum_{m=1}^{P+Q} d_m, \tag{61}$$

which is simply a Linear Program (LP).

We can then prove

Lemma 5.1. *For given* $\overline{\mu} \in \mathscr{V}^K$ *and* $\kappa \in \mathbb{R}^P$,

$$\hat{g}_{\overline{\mu}}(\mu; \kappa) \leqslant \overline{\beta}_{\overline{\mu}}(\mu) \quad \forall \mu \in \mathscr{D}. \tag{62}$$

Proof. We take as our point of departure the definition of $\overline{\beta}_{\overline{\mu}}(\mu)$, (50). We then write $T^{\mu} w$ as $T^{\overline{\mu}} w + (T^{\mu} w - T^{\overline{\mu}} w)$ and invoke (15) and (12) to obtain

$$\overline{\beta}_{\overline{\mu}}(\mu) = 1 + \inf_{w\in X} \left(\sum_{q=1}^{Q} (\Theta^q(\mu) - \Theta^q(\overline{\mu})) \frac{a^q(w, T^{\overline{\mu}} w)}{|||w|||^2_{\overline{\mu}}} \right). \tag{63}$$

Next, we add and subtract to our "infimand" in (63) the term

$$\sum_{q=1}^{Q} \sum_{p=1}^{P} \frac{\partial \Theta^q}{\partial \mu_p}(\overline{\mu}) \kappa_p (\mu_p - \overline{\mu}_p) \frac{a^q(w, T^{\overline{\mu}} w)}{|||w|||^2_{\overline{\mu}}}, \tag{64}$$

and group the contributions as

$$\begin{aligned} \overline{\beta}_{\overline{\mu}}(\mu) = 1 + \inf_{w\in X} \Bigg\{ & \sum_{p=1}^{P} \kappa_p (\mu_p - \overline{\mu}_p) \left(\sum_{q'=1}^{Q} \frac{\partial \Theta^{q'}}{\partial \mu_p}(\overline{\mu}) \frac{a^{q'}(w, T^{\overline{\mu}} w)}{|||w|||^2_{\overline{\mu}}} \right) \\ & + \sum_{q=1}^{Q} \left(\Theta^q(\mu) - \Theta^q(\overline{\mu}) - \sum_{p'=1}^{P} \frac{\partial \Theta^q}{\partial \mu_{p'}}(\overline{\mu}) \kappa_{p'} (\mu_{p'} - \overline{\mu}_{p'}) \right) \frac{a^q(w, T^{\overline{\mu}} w)}{|||w|||^2_{\overline{\mu}}} \Bigg\}. \end{aligned} \tag{65}$$

Finally, we note that the "inf of the sums" bounds from above the "sum of the infs"; we then invoke the equalities (58), (59), which concludes the proof. □

This proof is, of course, quite similar to the simpler "simplest affine" case.

As regards accuracy, we anticipate that (56) will inherit the good properties of the simple affine case to leading order; the general affine contributions only contribute to second order – and hence, even for larger Q, should be reasonably well controlled. We provide numerical evidence for this claim in Section 5.4.

Remark 3. We understand (from our "simplest affine" arguments) that our lower bound for $\overline{\beta}_{\overline{\mu}}(\mu)$ will be sharpest in the parameter coordinate directions. We can exploit the freedom in the parametric representation to "optimally" locally align a parameter coordinate with the largest gradients in $\overline{\beta}_{\overline{\mu}}(\mu = \overline{\mu})$. The derivatives of $\overline{\beta}_{\overline{\mu}}(\mu)$ and $\tilde{\beta}_{\overline{\mu}}(\mu)$ at $\mu = \overline{\mu}$ will only exist in the directional sense; however, we can plausibly assume – see the left inequality of (49) – that the steepest variation will be approximately aligned with the gradient of $\beta(\mu)$. Although $\beta(\mu)$ is not $C^1(\mathscr{D})$, the gradient $G(\mu) \in \mathbb{R}^P$ at $\mu = \overline{\mu}$ will generally exist, and can be formally evaluated by the usual sensitivity arguments as

$$G_p(\overline{\mu}) = \beta(\overline{\mu}) \sum_{q=1}^{Q} \frac{\partial \Theta^q}{\partial \mu_p}(\overline{\mu}) a^q(\chi(\overline{\mu}), T^{\overline{\mu}}\chi(\overline{\mu})), \quad p = 1, \ldots, P. \tag{66}$$

We may thus gainfully introduce, for given $\overline{\mu}$, a new parameter coordinate system $\hat{\mu} = R_{\overline{\mu}}\mu$ in which the first component of $\hat{\mu}$ aligns with $G(\overline{\mu})$; here $R_{\overline{\mu}} \in \mathbb{R}^{P\times P}$ is an orthogonal (rotation) matrix. We shall refer to the local lower bound construction based on μ – the parameter coordinate system given – as "without local rotation"; and the local lower bound construction based on $\hat{\mu}$ – the new parameter coordinate system optimally aligned – as "with local rotation." This rotation is of course a valid transformation independent of the rigor of the motivating arguments.

5.2.2. Global lower bound

For given $\mathscr{V}^K$, $\mathscr{I}^K$ our global lower bound function $g^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$: $\mathscr{D} \to \mathbb{R}$ is then given by

$$g^{\mathscr{V}^K,\mathscr{I}^K}(\mu) = g_{\mathscr{I}^K\mu}(\mu). \tag{67}$$

(Where there is no opportunity for confusion, we may abbreviate $g^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$ by $g^K(\mu)$.) We further define

$$g_{\min}^{\mathscr{V}^K,\mathscr{I}^K} = \min_{\mu\in\mathscr{D}} g^{\mathscr{V}^K,\mathscr{I}^K}(\mu). \tag{68}$$

We can then readily prove

Proposition 5.2. *For given* $\mathscr{V}^K, \mathscr{I}^K$,

$$g^{\mathscr{V}^K,\mathscr{I}^K}(\mu) \leqslant \tilde{\beta}^{\mathscr{V}^K,\mathscr{I}^K}(\mu) \quad \forall \mu \in \mathscr{D}. \tag{69}$$

Proof. The result follows directly from the definitions (55) and (67), Lemma 5.1, and the inequality (51). □

We note that $g_{\min}^{\mathscr{V}^K,\mathscr{I}^K}$ may be negative, in which case the lower bound is of little value.

We are also now in a position to return to – and prove – the stability of our adjoint deflation correction. In particular,

Proposition 5.3. *For* $\mathscr{V}^K, \mathscr{I}^K$ *such that* $g_{\min}^{\mathscr{V}^K,\mathscr{I}^K} > 0$, *the deflation correction* $\delta_{\overline{\mu}}(\mu)$ *defined in* (39), (40) *is bounded.*

Proof. We observe from (36), (10), (37), (15) and (48) that, for $\mu \in \mathscr{D}$ and $\overline{\mu} = \mathscr{I}^K\mu \in \mathscr{V}^K$,

$$r_N^{\mathrm{du},o}(\chi(\overline{\mu}); \mu) = a(\chi(\overline{\mu}), e^{\mathrm{du},o}(\mu); \mu) = (T^\mu\chi(\overline{\mu}), e^{\mathrm{du},o}(\mu))_X \leqslant \tilde{\gamma}_{\overline{\mu}}(\mu)\|T^{\overline{\mu}}\chi(\overline{\mu})\|_X \|e^{\mathrm{du},o}(\mu)\|_X. \tag{70}$$

We then note from (15), (39), (50), and (25) that

$$a(\chi(\overline{\mu}), \delta_{\overline{\mu}}(\mu); \mu) = c_{\overline{\mu}}(\mu)(T^\mu\chi(\overline{\mu}), T^{\overline{\mu}}\chi(\overline{\mu}))_X \geqslant c_{\overline{\mu}}(\mu)\overline{\beta}_{\overline{\mu}}(\mu)\|T^{\overline{\mu}}\chi(\overline{\mu})\|_X^2 = c_{\overline{\mu}}(\mu)\overline{\beta}_{\overline{\mu}}(\mu). \tag{71}$$

Therefore, it follows from (39), (25), (40), and Lemma 5.1, (67), (68) that

$$\|\delta_{\overline{\mu}}(\mu)\|_X \leqslant \frac{\tilde{\gamma}_{\overline{\mu}}(\mu)}{g_{\min}^{\mathscr{V}^K,\mathscr{I}^K}} \|e^{\mathrm{du},o}(\mu)\|_X, \tag{72}$$

which concludes the proof. □

5.3. Selection of $\mathscr{V}^K$, $\mathscr{I}^K$

We first discuss the choice of $\mathscr{I}^K$ given $\mathscr{V}^K$; we then discuss the construction of $\mathscr{V}^K$. For $\mathscr{I}^K$, the best choice will maximize our lower bound, $g^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$. It is thus clear that, given $\mathscr{V}^K$, we should specify $\mathscr{I}^K = \mathscr{I}^K_*$, where for given $\mu \in \mathscr{D}$,

$$\mathscr{I}^K_* \mu = \arg\max_{\overline{\mu}\in\mathscr{V}^K} g_{\overline{\mu}}(\mu). \tag{73}$$

In essence, (73) finds the best (largest) local lower bound. (We also expect, of course, that $\mathscr{I}^K_*\mu$ will be near μ in the usual Euclidean sense.) Equivalently, we may say that, for given $\mathscr{V}^K$, the choice $\mathscr{I}^K = \mathscr{I}^K_*$ maximizes $g_{\min}^{\mathscr{V}^K,\mathscr{I}^K}$ of (68) over all possible $\mathscr{I}^K$.

We conclude our development by proposing a procedure by which to determine a good set of parameter points $\mathscr{V}^K$ such that our lower bound is of value – $g_{\min}^{\mathscr{V}^K,\mathscr{I}^K}$ positive. We first introduce a large parameter sample $\Xi_g \subset \mathscr{D}$ of size $n^g \gg 1$. We next set $K = 1$ and select a tolerance $0 < g_{\mathrm{tol}} < 1$; we then choose $\overline{\mu}_1$, which in turn defines $g^{\mathscr{V}^1,\mathscr{I}^1_*}(\mu)$. We now proceed to calculate for $K = 1, \ldots,$

$$\overline{\mu}_{K+1} = \arg\max_{\mu\in\Xi_g} \left(\min_{\{\mu'\in\Xi_g | g^{\mathscr{V}^K,\mathscr{I}^K_*}(\mu') \geqslant g_{\mathrm{tol}}\}} |\mu - \mu'| \right) \tag{74}$$

until

$$\min_{\mu\in\Xi_g} g^{\mathscr{V}^K,\mathscr{I}^K_*}(\mu) \geqslant g_{\mathrm{tol}}; \tag{75}$$

here $|\cdot|$ refers to the usual Euclidean norm, though more general metrics may also be considered. In essence, (74) chooses the next point to be the farthest point from the "good set"; other approaches are certainly possible. Note that (75) does not quite ensure $g_{\min}^{\mathscr{V}^K,\mathscr{I}^K_*} \geqslant g_{\mathrm{tol}}$, since in (75) we consider only the finite albeit large sample $\Xi_g \subset \mathscr{D}$.

5.4. Numerical results

We demonstrate our lower bound first for Example I, the thermal plate fin problem of Section 3.1. We specify $n_g = 2000$ and $g_{\mathrm{tol}} = 0.5$ and apply ("without local rotation") the algorithm (74), (75) with (73) to obtain $\mathscr{V}^K$ and $\mathscr{I}^K_*$; we satisfy the desired tolerance for $K = 27$ – rather modest given the extensive parameter domain $\mathscr{D}$.

We present in Figs. 4(a) and (b) slices of $g^K(\mu) \equiv g^{\mathscr{V}^K,\mathscr{I}^K_*}(\mu)$ for $\mu_1 \equiv \alpha = 5$, $\mu_2 \equiv (\mathrm{Bi}\, L) = 0.1$, $\mu_3 \equiv L \in [2.5, 7.5]$, and for $\mu_1 \equiv \alpha = 1$, $\mu_2 \equiv (\mathrm{Bi}\, L) \in [0.05, 2.5]$, and $\mu_3 \equiv L = 5$, respectively.[4] We also include in Fig. 4 the sub-optimal non-scaled result

$$g^K_{\mathrm{ns}}(\mu) = \max_{\overline{\mu}\in\mathscr{V}^K} \hat{g}_{\overline{\mu}}(\mu; \kappa = (1 \quad 1 \quad 1)); \tag{76}$$

clearly, κ optimization – parameter rescaling – is quite effective in controlling the higher-order contributions.[5] Although our lower bound is in some sense rather low order, each local approximation is nevertheless valid – to the O(1) accuracy required for our error-bound purposes – over a considerable fraction of the parameter domain: the piecewise natural-norm inf–sup parameter is, by construction, a relatively simple function to represent.

[4] According to (73), $g^K(\mu)$ should be continuous. However in practice, to reduce online expense, we do not enumerate over all the $\overline{\mu} \in \mathscr{V}^K$ to evaluate $\mathscr{I}^K_*\mu$ – instead, the maximization process (73) is terminated once we find *any* $\overline{\mu} \in \mathscr{V}^K$ such that $g_{\overline{\mu}}(\mu) \geqslant g_{\mathrm{tol}}$.

[5] We note that for g^K_{ns} in (76) and Fig. 4 we retain $\mathscr{V}^K$ as calculated in (74), (75), (73) based on (67), (56); hence, $\mathscr{V}^K$ in (76) is optimized for $\kappa^{\mathrm{opt}}_{\overline{\mu}}(\mu)$ and *not* $\kappa = (1 \quad 1 \quad 1)$. Our comparison here is intended only to demonstrate the important effect of rescaling.

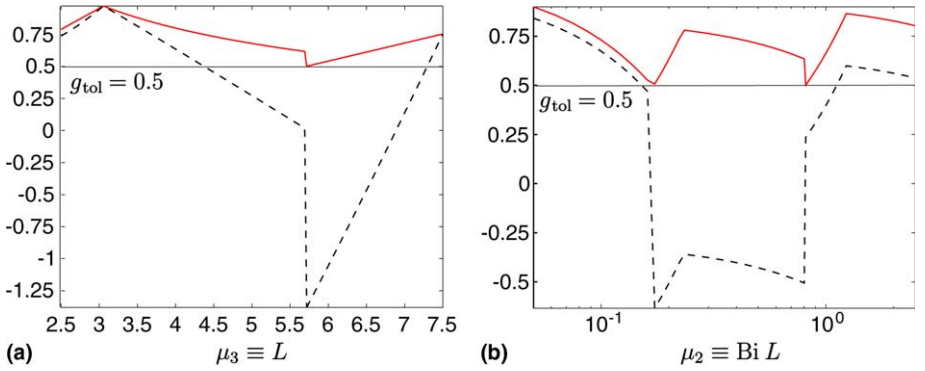

Fig. 4. Inf-sup lower bound for the Laplacian of Example I for (a) $\mu_1 \equiv \alpha = 5$, $\mu_2 \equiv \mathrm{Bi}\, L = 0.1$, $\mu_3 \equiv L \in [2.5, 7.5]$, and (b) $\mu_1 \equiv \alpha = 1$, $\mu_2 \equiv \mathrm{Bi}\, L \in [0.05, 2.5]$, $\mu_3 \equiv L = 5$. We present both $g^K(\mu)$ (solid line) and $g^K_{\rm ns}(\mu)$ (dashed line).

Table 3
Requisite sample size of $\mathscr{V}^K$ for $g_{\rm tol} = 0.5$ for the Helmholtz problem of Example II without (K) and with ($K_{\rm PP}$) Post-Processing

Case	Rotation	κ optimization	K	$K_{\rm PP}$
1	Yes	Yes	14	8
2	No	Yes	18	15
3	Yes	No	18	15
4	No	No	21	20

We next demonstrate our lower bound for Example II, the acoustics Helmholtz problem of Section 3.2. We specify a uniform grid $\Xi_g \subset \mathscr{D}$ of size $n_g = 3200$ and prescribe $g_{\rm tol} = 0.5$. We now apply our algorithm (74), (75) with (73) both "with local rotation" and "without local rotation" (see Remark 3), and both "with κ optimization" and "without κ optimization"; in the "without κ optimization" case, we replace $g_{\overline{\mu}}(\mu)$ of (56) with $\hat{g}_{\overline{\mu}}(\mu; \kappa = (1 \quad 1))$. The four cases considered are defined in Table 3. Note that for each case considered the parameter set $\mathscr{V}^K$ (and hence also $\mathscr{I}^K_*$) is chosen optimally for the particular case. In each case we also pursue a simple Post-Processing step[6] in which we eliminate unnecessary points that are artifacts of our greedy algorithm – since our procedure to determine the set of parameter points $\mathscr{V}^K$ is not necessarily optimal, it is likely that there are some redundant points in $\mathscr{V}^K$.

Our results for Cases 1–4 are summarized in Table 3 in terms of the requisite K and $K_{\rm PP}$ (Post-Processed) for the given $g_{\rm tol} = 0.5$. (Recall that $\mathscr{V}^K$, $\mathscr{I}^K_*$, and K are optimized and hence different for each case.) We show in Fig. 5 the parameter set $\mathscr{V}^K$ for Case 1 ("with local rotation" and "with κ optimization") without Post-Processing. Clearly, κ optimization, local rotation, and Post-Processing can, in concert, significantly reduce the requisite sample size. We observe however that, although K is quite modest, there is indeed a concentration of points in $\mathscr{V}^K$ near the resonance curve; this is necessary in order to accommodate the second-order or "curvature" contributions to the inf–sup parameter. This does imply some significant dependence of K on P (the number of parameters) since in general the resonance curves will be $(P-1)$-dimensional manifolds. In order to quantify this effect, and also the mitigating effect of any damping, further tests in higher parameter dimensions are required [28].

6. A posteriori error estimation

6.1. Formulation

We first introduce a bound for the natural norm of the primal error; we then turn to the error bound for the output of interest. Throughout this section, we presume that $g^K(\mu) \equiv g^{\mathscr{V}^K, \mathscr{I}^K}(\mu)$ for given $\mathscr{V}^K$ and $\mathscr{I}^K$ (typically $\mathscr{I}^K_*$); and that $g^K_{\min} \equiv g^{\mathscr{V}^K, \mathscr{I}^K}_{\min}$ of (68) is positive.

[6] To Post Process $\mathscr{V}^K$ we consider each point $\overline{\mu}_k$, $1 \leqslant k \leqslant K$, in turn; we eliminate the point if the resulting reduced sample preserves our $g_{\rm tol}$ requirement.

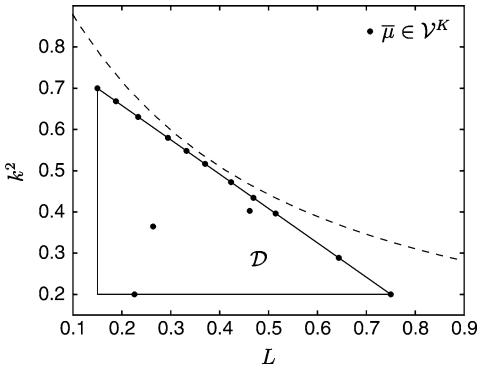

Fig. 5. Parameter sample $\mathcal{V}^K$ for the Helmholtz problem of Example II for Case 1 ("with local rotation"and "with κ optimization") without Post-Processing. The dashed line indicates the (first) resonance curve.

Our bound for the primal error in the natural norm is given by

$$\Delta_N(\mu) \equiv \frac{1}{g^K(\mu)} \|r_N^{\rm pr}(\cdot;\mu)\|_{X'}, \tag{77}$$

where the dual norm is defined in (13). We can prove

Lemma 6.1. *For given $\mu \in \mathcal{D}$, the primal error satisfies*

$$|||e^{\rm pr}(\mu)|||_{\overline{\mu}} \leqslant \Delta_N(\mu), \tag{78}$$

where $\overline{\mu} = \mathcal{I}^K \mu$.

Proof. It follows from the error-residual relationship, $a(e^{\rm pr}(\mu), v; \mu) = r_N^{\rm pr}(v;\mu)$, $\forall v \in X$, the inf–sup definition (47), (55), and Proposition 5.2, that

$$g^K(\mu)|||e^{\rm pr}(\mu)|||_{\overline{\mu}} \|T^\mu e^{\rm pr}(\mu)\|_X \leqslant |r_N^{\rm pr}(T^\mu e^{\rm pr}(\mu);\mu)|. \tag{79}$$

But clearly, from (13), $|r_N^{\rm pr}(T^\mu e^{\rm pr}(\mu);\mu)|/\|T^\mu e^{\rm pr}(\mu)\|_X \leqslant \|r_N^{\rm pr}(\cdot;\mu)\|_{X'}$, which concludes the proof. □

We can also readily demonstrate that

$$\Delta_N(\mu) \leqslant \frac{\gamma_{\overline{\mu}}(\mu)}{g^K(\mu)} |||e^{\rm pr}(\mu)|||_{\overline{\mu}}; \tag{80}$$

however this good effectivity in the natural norm is not yet relevant to our ultimate objective – a bound for the error in the output of interest.

We shall require one additional preliminary result, which we provide in

Lemma 6.2. *For a functional $h \in X'$ that, for a given $\overline{\mu} \in \mathcal{V}^K$, satisfies $h(\chi(\overline{\mu})) = 0$,*

$$\sup_{v \in X} \frac{h(v)}{|||v|||_{\overline{\mu}}} \leqslant \frac{1}{\beta^+(\overline{\mu})} \|h\|_{X'}. \tag{81}$$

Proof. We first observe by standard duality arguments that

$$\sup_{v \in X} \frac{h(v)}{|||v|||_{\overline{\mu}}} = \frac{h(H)}{|||H|||_{\overline{\mu}}}, \tag{82}$$

where, from the definition (18), $(T^{\overline{\mu}}H, T^{\overline{\mu}}v)_X = h(v)\ \forall v \in X$. It is clear from our hypothesis on h that

$$(T^{\overline{\mu}}H, T^{\overline{\mu}}\chi(\overline{\mu}))_X = 0. \tag{83}$$

We now expand H as

$$H = \sum_{i=1}^{\mathcal{N}_t} c_i \Phi_i(\overline{\mu}), \tag{84}$$

and observe from (21), (25), and the orthogonality condition (83) that $c_1 = 0$. We further note from (19), (21), and (24) that

$$|||H|||_{\overline{\mu}}^2 = \sum_{i=1}^{\mathcal{N}_t} c_i^2 \rho_i(\overline{\mu}) = \sum_{i=2}^{\mathcal{N}_t} c_i^2 \rho_i(\overline{\mu}) \geqslant (\beta^+(\overline{\mu}))^2 \sum_{i=2}^{\mathcal{N}_t} c_i^2 = (\beta^+(\overline{\mu}))^2 \|H\|_X^2. \tag{85}$$

Therefore, from (85) and (13),

$$\frac{h(H)}{|||H|||_{\overline{\mu}}} \leqslant \frac{h(H)}{\beta^+(\overline{\mu})\|H\|_X} \leqslant \frac{1}{\beta^+(\overline{\mu})} \|h\|_{X'}, \tag{86}$$

which concludes the proof. □

This lemma is not surprising: it is a standard norm-equivalence argument except that we have eliminated the extreme mode.

We now define our output error bound as

$$\Delta_N^s(\mu) \equiv \frac{1}{\beta^+(\overline{\mu}) g^K(\mu)} \|r_N^{\mathrm{du}}(\cdot;\mu)\|_{X'} \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'} \tag{87}$$

for $\overline{\mu} = \mathscr{I}^K \mu$. We can then prove

Proposition 6.3. *The output error satisfies*

$$|s(\mu) - s_N(\mu)| \leqslant \Delta_N^s(\mu) \quad \forall \mu \in \mathscr{D}. \tag{88}$$

Proof. We first observe from Lemmas 4.1 and 6.1 that, for $\overline{\mu} = \mathscr{I}^K \mu$,

$$|s(\mu) - s_N(\mu)| = |r_N^{\mathrm{du}}(e^{\mathrm{pr}}(\mu);\mu)| \leqslant \left(\sup_{v \in X} \frac{r_N^{\mathrm{du}}(v;\mu)}{|||v|||_{\overline{\mu}}} \right) |||e^{\mathrm{pr}}(\mu)|||_{\overline{\mu}} \leqslant \left(\sup_{v \in X} \frac{r_N^{\mathrm{du}}(v;\mu)}{|||v|||_{\overline{\mu}}} \right) \Delta_N(\mu). \tag{89}$$

We now observe from (38), (40) and (41) that $r_N^{\mathrm{du}}(\chi(\overline{\mu});\mu) = 0$, and hence from Lemma 6.2

$$\sup_{v \in X} \frac{r_N^{\mathrm{du}}(v;\mu)}{|||v|||_{\overline{\mu}}} \leqslant \frac{1}{\beta^+(\overline{\mu})} \|r_N^{\mathrm{du}}(\cdot;\mu)\|_{X'}, \tag{90}$$

which concludes the proof. □

We note that Proposition 6.3 is valid for any N_{pr}, N_{du}.

The quality, or sharpness, of our output bound is measured by the effectivity,

$$\eta_N^s(\mu) \equiv \frac{\Delta_N^s(\mu)}{|s(\mu) - s_N(\mu)|}. \tag{91}$$

In general, we cannot bound this output effectivity. The incorporation of the dual in the bound does eliminate one important source of deterioration in the effectivity, in which (in particular, as ℓ approaches f) the primal space well approximates the dual solution – and hence the output converges faster than the primal error even without the dual correction [15]. However, another source of deterioration in the effectivity remains: implicitly, our bound in (87) ignores any possible de-correlation between the primal and dual errors – whereas in fact $|s(\mu) - s_N(\mu)|$ may be significantly smaller than the product of the primal and dual errors. We can thus hope that our effectivities will be well-behaved, but this may not always be the case [15]. We do note that, given the rapid convergence of the reduced basis approximation, O(10) effectivities are not particularly worrisome, as this can readily be absorbed by only a very slight increase in N.

Deflation can also play an important role in controlling effectivities. In particular, many coercive and non-coercive problems may exhibit near singular behavior in which $\beta(\mu)$ tends to zero: this occurs in Example I, the

thermal fin/Laplacian, as we approach the Bi = 0 boundary of $\mathcal{D}$; this also occurs in Example II, the acoustic "microphone probe"/Helmholtz, as we approach resonances just outside $\mathcal{D}$ (or more generally, for lightly damped systems, *at* resonances within $\mathcal{D}$). Without deflation we must accommodate $1/\beta(\overline{\mu})$ in the denominator of our error bound – the worst mode "pollutes" the estimate for all the modes; with deflation, we are permitted the much more benign $1/\beta^+(\overline{\mu})$ in the denominator of our error bound – since the most dangerous mode has now been "peeled off." Clearly, our arguments assume that there is only one dangerous mode (or, with suitable generalization, some small finite number of dangerous modes), as obtains in both the examples cited: if there are *no* dangerous modes, deflation is an unnecessary expense; if there are *many* (a continuum of) dangerous modes, deflation cannot be effective. The former is benign; the latter is unlikely – an indication of fundamental ill-posedness.

Remark 4. In the case of compliance (see Remark 1) – a symmetric and $\ell = f$ – we replace our output error bound (87) with

$$\Delta_N^s(\mu) \equiv \frac{1}{\beta^+(\overline{\mu})g^K(\mu)} \|r_N^{\mathrm{du}}(\cdot;\mu)\|_{X'}^2 \quad \text{(compliant)}; \tag{92}$$

recall that we no longer require the primal solution. If we additionally require coercivity of a, we can in fact bound the effectivity (since now the output error can be zero only if the dual error is zero):

$$\eta_N^s(\mu) \leqslant \frac{\gamma(\mu)}{\beta^+(\overline{\mu})g^K(\mu)} \quad \text{(compliant, coercive)}, \tag{93}$$

which is similar to the standard result [7] but now corrected for deflation. Here $\overline{\mu} = \mathscr{I}^K\mu$ in both (92) and (93).

Remark 5. There are error indicator proposals in other contexts – adaptive finite difference techniques for ordinary differential equations [33] and adaptive finite element methods for partial differential equations [30] – that do not require an explicit lower bound for the stability constant. These indicators are intended primarily for adaptive refinement, not certification.

In our context, the indicator in [33] (might) take the form

$$\widehat{\Delta}_N^s(\mu) \equiv \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'}\|\psi_N^o(\mu)\|_X$$

as motivated by the relation

$$|\ell(u(\mu) - u_N(\mu))| \leqslant \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'}\|\psi(\mu)\|_X \leqslant \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'}(\|\psi_N^o(\mu)\|_X + \|e^{\mathrm{du},0}(\mu)\|_X) \approx \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_{X'}\|\psi_N^o(\mu)\|_X.$$

Clearly, $\widehat{\Delta}_N^s(\mu)$ is not a rigorous upper bound for $|\ell(u(\mu) - u_N(\mu))|$, and hence is not too well suited for certification; in essence, the stability constant is hidden (albeit to second order [30]) in the neglected adjoint error term. In our particular context, control of the effectivity may also be compromised, as Galerkin orthogonality is not recognized: for example, in the compliance case, $\widehat{\Delta}_N^s(\mu)/|\ell(u(\mu) - u_N(\mu))|$ will tend to infinity as N increases. Finally, there is also an efficiency issue: if we calculate $\psi_N(\mu)$, we should include the residual correction term in (43) – to improve the output accuracy [31]; but the associated error indicator will then be consistent only if we now bound the adjoint *error* – which again requires a stability constant.

In our context, the indicators in [30] (might) take the form (for $s_N(\mu)$ as defined in (43))

$$|s(\mu) - s_N(\mu)| \approx \|r_N^{\mathrm{pr}}(\cdot;\mu)\|_X\|\psi_{2N}^o(\mu) - \psi_N^o(\mu)\|_X,$$

where $\psi_{2N}^o(\mu)$ and $\psi_N^o(\mu)$ refer to our reduced basis dual approximation for $2N_{\mathrm{du}}$ and N_{du} dual basis functions, respectively. Again, this indicator does not provide a rigorous bound; however, the treatment of the adjoint error would at least partially address both the effectivity and efficiency/accuracy concerns.

6.2. Numerical results

We present in Table 1 the error bounds and effectivities for the two outputs $s_1(\mu)$ and $s_2(\mu)$ – associated with the output functionals $\ell_1(\mu)$ and $\ell_2(\mu)$, respectively – for Example I of Section 3.1, the thermal plate fin. As

before, we present the results in terms of $N_{\rm du}$; for the first (compliant) output, there is no need for a primal solution – we invoke (92); for the second (non-compliant) output, we take $N_{\rm pr} = N_{\rm du}$. The error bound $\mathscr{E}_{i,N}$ reported for each output, subscript $i = 1, 2$, is the maximum of the relative error bound, $|\Delta^s_{i,N}(\mu)|/|s_i(\mu)|$, over our random parameter test sample $\Xi^{\rm I}_{\rm test} \subset \mathscr{D}$ of size $n^{\rm I}_{\rm test} = 1000$; for each output, subscript $i = 1, 2, \overline{\eta}^s_{i,N}$ denotes the average of the effectivity, $\eta^s_{i,N}(\mu)$, over the parameter test sample $\Xi^{\rm I}_{\rm test}$. (Note that we reject from our sample $\Xi^{\rm I}_{\rm test}$ those parameter points for which the dual norm of the residual squared is smaller than machine precision, as for these parameter points the calculation is contaminated by round-off.)

We observe – though we cannot a priori guarantee – reasonably good effectivities for both the compliant and non-compliant outputs. Note that, without deflation, the *error* in the reduced basis output prediction changes only imperceptibly. However, for the lower $\mu_2 \equiv (\mathrm{Bi}\, L)$ values – $\mathrm{Bi} \in [0.01, 0.1]$ – the without-deflation output *error bound*, (87) but with $\beta^+(\mu)$ replaced by $\beta(\overline{\mu})$ in the denominator, is approximately *80 times larger* than the with-deflation output error bound $\Delta^s_N(\mu)$: deflation is a necessity for nearly singular problems if we wish to control the effectivity.

We present in Table 2 the error bounds and effectivity for the (non-compliant) output of Example II of Section 3.2, the acoustics Helmholtz problem. As before, we present the results in terms of $N_{\rm du}$ ($=N_{\rm pr}$). The error bound $\mathscr{E}_N$ is the maximum of the relative error bound, $|\Delta^s_N(\mu)|/|s(\mu)|$, over our random parameter test sample $\Xi^{\rm II}_{\rm test} \subset \mathscr{D}$ of size $n^{\rm II}_{\rm test} = 400$; $\overline{\eta}^s_N$ is the average of the effectivity, $\eta^s_N(\mu)$, over the parameter test sample $\Xi^{\rm II}_{\rm test}$. (As before, we reject from our sample $\Xi^{\rm II}_{\rm test}$ those parameter points for which the dual norm of the residual squared is smaller than machine precision.) We observe reasonably good effectivities. Near resonance, the without-deflation output error bound is approximately *10–40 times larger* than the with-deflation output error bound: deflation is a necessity for Helmholtz problems near resonance.

7. Computational cost: offline/online approach

Our reduced basis approach admits an offline/online computational decomposition [6,7,9,10,12]: all $\mathscr{N}_t$-dependent operations are first performed *offline* in a preprocessing stage; the computational complexity and storage of the *online* – or "deployed" – stage then depends only on N, Q, and K. In the online stage we can provide extremely rapid response in the real-time context, and extremely efficient (average) response in the many-query context; an example of both the former and the latter is the "non-destructive evaluation" parameter estimation framework described briefly in Section 1.2 and illustrated in detail in [16,18,22].

The total online cost for the output and output error bound, inclusive of both the primal and dual solutions, the deflation correction, the inf–sup lower bound, and the dual norms of the primal and dual residuals, is $\mathrm{O}(N^3_{\rm pr} + N^3_{\rm du} + Q^2(N_{\rm pr} + N_{\rm du} + 1)^2)$. The storage scales as $\mathrm{O}(Q^2(N^2_{\rm pr,max} + N^2_{\rm du,max} + KN_{\rm du,max}))$.[7] Thus, all requisite online calculations and storage are indeed *independent* of the dimension of the underlying finite element space, $\mathscr{N}_t$. A detailed accounting of the online operation count and storage is presented in Appendix A.

We now compare the online reduced basis computational cost to evaluate $s_N(\mu)$ and $\Delta^s_N(\mu)$ to the finite element cost to compute our "truth" output $s(\mu) \equiv s^{\mathscr{N}_t}(\mu)$. Of course, this comparison is only meaningful if we are in the real-time or many-query contexts – in which the offline reduced basis cost is unimportant, and only the marginal cost is relevant. We present our results in Table 4 for Example I and Table 5 for Example II.[8] Note we do not necessarily observe the expected scalings with $N_{\rm du}$ due to memory access and other overhead not accounted for in our complexity estimates.

We conclude from Table 1/Table 4 and Table 2/Table 5 that, for both our model problems, our approach provides *certified* relative accuracy of 10^{-3} or 10^{-4} at (1/100)th the online cost of conventional techniques. The

[7] We have chosen to express our output error bound (87) in terms of X' dual norms, which in turn necessitates deflation in order to ensure good effectivities (see (90) and the discussion following Proposition 6.3). An alternative (see (89)) is to work directly with natural dual norms and "hope" that the most dangerous mode is largely absent; however, this natural dual norm approach could incur larger effectivities and, in any event, will require $\mathrm{O}(KQ^2N^2_{\rm du,max})$ online storage – typically a K-fold increase over the X' dual norm approach presented.

[8] The online times are exclusive of the inf–sup lower bound calculation, which in our normalized units is (say, for Example I) about 9.77 (independent of $N_{\rm du}$ and of course $\mathscr{N}_t$). A more efficient LP strategy for κ optimization could reduce this overhead.

Table 4
Example I, Thermal plate fin: computational cost to evaluate $s_{1,N}$, $\Delta^s_{1,N}$, $s_{2,N}$, $\Delta^s_{2,N}$, and $s^{\mathcal{N}_t}$ as a function of N_{du} (for $N_{pr} = N_{du}$); the results are normalized with respect to the time to calculate $s_{1,N}$ for $N_{du} = 4$

N_{du}	Online time				Time
	$s_{1,N}$	$\Delta^s_{1,N}$	$s_{2,N}$	$\Delta^s_{2,N}$	$s^{\mathcal{N}_t}$
4	1.00	5.37	1.42	5.58	
8	1.16	5.42	1.68	5.74	
12	1.26	5.63	1.89	6.00	2000
16	1.42	5.84	2.00	6.05	
20	–	–	2.16	6.58	

Table 5
Example II, "Microphone probe": computational cost to evaluate s_N, Δ^s_N, and $s^{\mathcal{N}_t}$ as a function of N_{du} (for $N_{pr} = N_{du}$); the results are normalized with respect to the time to calculate s_N for $N_{du} = 2$

N_{du}	Online time		Time
	s_N	Δ^s_N	$s^{\mathcal{N}_t}$
2	1	1.5	
4	1.07	1.5	
6	1.14	1.58	1800
8	1.21	1.58	
10	1.22	1.58	

savings would be even larger for problems with more complex geometry and solution structures, and in particular in higher space dimensions with correspondingly larger $\mathcal{N}_t$.

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Appendix A. Offline/online computational procedures

In this appendix we develop the offline/online computational decomposition which allows us to efficiently compute the primal and dual solutions, the output, and the error bounds in the online (or "deployed") stage. In particular, we outline the procedure to compute the deflated dual solution $\psi_N(\mu)$, the inf–sup lower bound $g^K(\mu)$, the output $s_N(\mu)$, and the dual norm of the dual residual $\|r^{du}_N(\cdot;\mu)\|_{X'}$. Similar computational procedures can be developed for the primal solution $u_N(\mu)$ and the dual norm of the primal residual $\|r^{pr}_N(\cdot;\mu)\|_{X'}$. For simplicity, we shall assume in this appendix a and a^q, $1 < q < Q$, are symmetric.

A.1. Calculation of $\psi_N(\mu)$

The deflated dual approximation ψ_N is a sum of the "undeflated" dual approximation $\psi^o_N(\mu)$, (35), and the deflation correction term $\delta_{\overline{\mu}}(\mu)$, (39).

We first express the "undeflated" dual approximation $\psi^o_N(\mu)$ as

$$\psi^o_N(\mu) = \sum_{j=1}^{N_{du}} \psi^o_{Nj}(\mu)\zeta^{du}_j. \tag{A.1}$$

We then choose as test functions $v = \zeta^{du}_i, i = 1,\ldots,N_{du}$, to represent our dual problem (35) algebraically: find $\underline{\psi}^o_N(\mu) \in \mathbb{R}^{N_{du}}$ such that

$$\underline{A}^{du}_N(\mu)\underline{\psi}^o_N(\mu) = -\underline{L}^{du}_N. \tag{A.2}$$

Here $\underline{\psi}^o_N = (\psi^o_{N1} \cdots \psi^o_{NN_{\rm du}})$, $\underline{A}^{\rm du}_N(\mu) \in \mathbb{R}^{N_{\rm du}\times N_{\rm du}}$ is the symmetric matrix $A^{\rm du}_{Ni,j}(\mu) \equiv a(\zeta^{\rm du}_j, \zeta^{\rm du}_i; \mu), 1 \leqslant i,j \leqslant N_{\rm du}$, and $\underline{L}^{\rm du}_N \in \mathbb{R}^{N_{\rm du}}$ is the "output" vector $L^{\rm du}_{Ni} \equiv \ell(\zeta^{\rm du}_i), i = 1,\ldots,N_{\rm du}$.

We now invoke the affine decomposition (12) to obtain

$$A^{\rm du}_{Ni,j}(\mu) = a(\zeta^{\rm du}_j, \zeta^{\rm du}_i; \mu) = \sum_{q=1}^{Q} \Theta^q(\mu) a^q(\zeta^{\rm du}_j, \zeta^{\rm du}_i), \tag{A.3}$$

which can be written as

$$\underline{A}^{\rm du}_N(\mu) = \sum_{q=1}^{Q} \Theta^q(\mu) \underline{A}^{{\rm du},q}_N, \tag{A.4}$$

where the $\underline{A}^{{\rm du},q}_N \in \mathbb{R}^{N_{\rm du}\times N_{\rm du}}$ are given by $A^{{\rm du},q}_{Ni,j} = a^q(\zeta^{\rm du}_j, \zeta^{\rm du}_i), 1 \leqslant i,j \leqslant N_{\rm du}, 1 \leqslant q \leqslant Q$.

The coefficient for the deflation correction $c_{\overline{\mu}}(\mu)$, (39), can then be calculated from (40) (for given $\overline{\mu}_k \in \mathscr{V}^K$) as

$$c_{\overline{\mu}}(\mu) \sum_{q=1}^{Q} \Theta^q(\mu) C^{q,k} = -L^k_\chi - \sum_{q=1}^{Q} \Theta^q(\mu) \left(\underline{D}^{{\rm du},q,k}_N\right)^{\rm T} \underline{\psi}^o_N(\mu), \tag{A.5}$$

where the *parameter-independent* quantities $C^{q,k}, L^k_\chi$, and $\underline{D}^{{\rm du},q,k}$ are given by

$$\begin{aligned} C^{q,k} &= a^q(\chi(\overline{\mu}_k), T^{\overline{\mu}_k}\chi(\overline{\mu}_k)), \quad 1 \leqslant k \leqslant K,\ 1 \leqslant q \leqslant Q, \\ L^k_\chi &= \ell(\chi(\overline{\mu}_k)), \quad 1 \leqslant k \leqslant K, \\ D^{{\rm du},q,k}_{N,i} &= a^q(\chi(\overline{\mu}_k), \zeta^{\rm du}_i), \quad 1 \leqslant k \leqslant K,\ 1 \leqslant q \leqslant Q,\ 1 \leqslant i \leqslant N_{\rm du,max}, \end{aligned} \tag{A.6}$$

respectively. Here $^{\rm T}$ denotes algebraic transpose.

The offline/online decomposition is now clear. In the *offline* stage – performed only once – we first solve for the $\zeta^{\rm du}_n, 1 \leqslant n \leqslant N_{\rm du,max}$; we then compute and store the μ-independent quantities in (A.2), (A.4) and (A.6). The computational cost is therefore $O(N_{\rm du,max})$ solutions of the underlying $\mathscr{N}_{\rm t}$-dimensional "truth" finite element approximation and $O(Q(N^2_{\rm du} + KN_{\rm du}))$ $\mathscr{N}_{\rm t}$-inner products.

In the *online* stage – performed many times, for each new parameter μ (and hence associated $\overline{\mu} = \mathscr{I}^K\mu \in \mathscr{V}^K$, which determines k in (A.5)) – we first assemble the reduced basis matrix (A.4); this requires $O(Q(N^2_{\rm du}))$ operations. We then solve the dual problem for $\underline{\psi}^o_N(\mu)$; since the reduced basis matrices are in general full, the operation count (based on LU factorization) is $O(N^3_{\rm du})$. Finally, we solve for $c_{\overline{\mu}}(\mu)$; this requires $O(QN_{\rm du})$ operations. The total online storage cost is $O(QN^2_{\rm du,max}) + O(KQN_{\rm du,max})$.[9]

A.2. Calculation of $g^{\mathscr{V}^K,\mathscr{I}^K}(\mu)$

We consider here only the online stage. For a particular given (new) μ, we must solve at most K Linear Programs of the form (56) (or (60), (61)) with $O(P+Q)$ variables and constraints. Typically, many fewer than K LPs are required: to wit (see Footnote 4), we first list the $\overline{\mu} \in \mathscr{V}^K$ in order of increasing distance from μ; we then proceed through this re-ordered list until we find a $\overline{\mu}$ such that $g_{\overline{\mu}}(\mu) \geqslant g_{\rm tol}$.

A.3. Calculation of $s_N(\mu)$

The output (43) can be calculated in terms of $\underline{u}_N(\mu) \in \mathbb{R}^{N_{\rm pr}}$, $\underline{\psi}^o_N(\mu) \in \mathbb{R}^{N_{\rm du}}$, and $c_{\overline{\mu}}(\mu)$, as

$$s_N(\mu) = \underline{L}^{{\rm pr}\,{\rm T}}_N \underline{u}_N(\mu) - \underline{F}^{{\rm du}\,{\rm T}}_N \underline{\psi}_N(\mu) + \sum_{q=1}^{Q} \Theta^q(\mu) \left(\underline{\psi}^o_N(\mu)^{\rm T} \underline{A}^{{\rm pr,du},q}_N \underline{u}_N(\mu) + c_{\overline{\mu}}(\mu) (\underline{B}^{{\rm pr},q,k}_N)^{\rm T} \underline{u}_N(\mu) \right), \tag{A.7}$$

where $\underline{u}_N(\mu) = (u_{N1} \cdots u_{NN_{\rm pr}})$ are the primal coefficients in the expansion $u_N(\mu) = \sum_{i=1}^{N_{\rm pr}} u_{Ni}(\mu)\zeta^{\rm pr}_i$, and k is the index of $\mathscr{I}^K\mu \in \mathscr{V}^K$. The *parameter-independent* quantities $\underline{L}^{\rm pr}_N$, $\underline{F}^{\rm du}_N$, $\underline{A}^{\rm pr,du,q}_N$, and $\underline{B}^{{\rm pr},q}_N$ are given by

[9] Recall $N_{\rm du,max}$ is the maximum size of the dual approximation space; $N_{\rm du,max}$ is independent of the size of the finite element mesh $\mathscr{N}_{\rm t}$. Section 4 and Footnote 3 summarize the construction of the primal and dual reduced basis spaces.

$$
\begin{aligned}
L^{\mathrm{pr}}_{Nj} &= \ell(\zeta^{\mathrm{pr}}_j), \quad 1 \leqslant j \leqslant N_{\mathrm{pr}},\\
F^{\mathrm{du}}_{Ni} &= \ell(\zeta^{\mathrm{du}}_i), \quad 1 \leqslant i \leqslant N_{\mathrm{du}},\\
A^{\mathrm{pr,du}}_{Ni,j} &= a^q(\zeta^{\mathrm{pr}}_j, \zeta^{\mathrm{du}}_i), \quad 1 \leqslant q \leqslant Q,\ 1 \leqslant i \leqslant N_{\mathrm{du,max}},\ 1 \leqslant j \leqslant N_{\mathrm{pr,max}},\\
B^{\mathrm{pr},q,k}_{N,i} &= a^q(\zeta^{\mathrm{pr}}_i, T^{\overline{\mu}_k}\chi(\overline{\mu}_k)), \quad 1 \leqslant k \leqslant K,\ 1 \leqslant q \leqslant Q,\ 1 \leqslant i \leqslant N_{\mathrm{pr,max}},
\end{aligned}
\tag{A.8}
$$

respectively.

In the *offline* stage, the operation count to construct the terms in (A.8) is $O(QN_{\mathrm{pr}}(N_{\mathrm{du}} + K))$ $\mathcal{N}_t$-inner products. In the *online* stage – for any new parameter μ – the output evaluation (43) requires $O(QN_{\mathrm{pr}}N_{\mathrm{du}})$ operations; the online storage is $O(KQN_{\mathrm{pr,max}}) + O(QN_{\mathrm{pr,max}}N_{\mathrm{du,max}})$.

A.4. Calculation of $\|r^{\mathrm{du}}_N(\cdot;\mu)\|_{X'}$

In this section we discuss the calculation of the dual norm of the dual residual. We first note from standard duality arguments that

$$
\|r^{\mathrm{du}}_N(\cdot;\mu)\|_{X'} \equiv \sup_{v\in X} \frac{r^{\mathrm{du}}_N(v;\mu)}{\|v\|_X} = \|\hat{e}^{\mathrm{du}}(\mu)\|_X
\tag{A.9}
$$

where $\hat{e}^{\mathrm{du}}(\mu) \in X$ is given by

$$
(\hat{e}^{\mathrm{du}}(\mu), v)_X = r^{\mathrm{du}}_N(v;\mu) \quad \forall v \in X.
\tag{A.10}
$$

From (41) and the affine assumption (12) it thus follows that $\hat{e}^{\mathrm{du}}(\mu)$, for any choice of $\overline{\mu}_k \in \mathcal{V}^K, 1 \leqslant k \leqslant K$, satisfies

$$
(\hat{e}^{\mathrm{du}}(\mu), v)_X = -\ell(v) - \sum_{j=1}^{N_{\mathrm{du}}}\sum_{q=1}^{Q} \Theta^q(\mu)\psi^o_{Nj}(\mu)a^q(\zeta^{\mathrm{du}}_j, v) - \sum_{q=1}^{Q}\Theta^q(\mu)c_{\overline{\mu}}(\mu)a^q(v, T^{\overline{\mu}_k}\chi(\overline{\mu}_k)) \quad \forall v \in Y.
\tag{A.11}
$$

It is clear from linear superposition that we can express $\hat{e}^{\mathrm{du}}(\mu)$ as

$$
\hat{e}^{\mathrm{du}}(\mu) = \hat{z}_0 - \sum_{q=1}^{Q}\sum_{j=1}^{N_{\mathrm{du}}} \Theta^q(\mu)\psi^o_{Nj}(\mu)\hat{z}^{\mathrm{du},q}_j - \sum_{q=1}^{Q}\Theta^q(\mu)c_{\overline{\mu}}(\mu)\hat{x}^q_k,
\tag{A.12}
$$

where $\hat{z}_0 \in X$, $\hat{z}^{\mathrm{du},q}_j \in X$, $\hat{x}^q_k \in X, 1 \leqslant k \leqslant K, 1 \leqslant q \leqslant Q, 1 \leqslant j \leqslant N_{\mathrm{du,max}}$, satisfy

$$
\begin{aligned}
(\hat{z}_0, v)_X &= -\ell(v) \quad \forall v \in X,\\
(\hat{z}^{\mathrm{du},q}_j, v)_X &= a^q(v, \zeta^{\mathrm{du}}_j) \quad \forall v \in X,\ 1 \leqslant q \leqslant Q,\ 1 \leqslant j \leqslant N_{\mathrm{du,max}},\\
(\hat{x}^q, v)_X &= a^q(T^{\overline{\mu}_k}\chi(\overline{\mu}_k), v) \quad \forall v \in X,\ 1 \leqslant k \leqslant K,\ 1 \leqslant q \leqslant Q.
\end{aligned}
\tag{A.13}
$$

Note that $\hat{z}_0$, $\hat{z}^{\mathrm{du},q}_j$, and $\hat{x}^q_k$ are *parameter independent*.

From (A.9) and (A.12) it follows that (for given k)

$$
\begin{aligned}
\|r^{\mathrm{du}}_N(\cdot;\mu)\|^2_{X'} = {} & \Lambda^{\mathrm{du},bb} + \sum_{q=1}^{Q}\sum_{j=1}^{N_{\mathrm{du}}} \Theta^q(\mu)\psi^o_{Nj}(\mu)\Lambda^{\mathrm{du},ab}_{q,j} + \sum_{q=1}^{Q}\Theta^q(\mu)c_{\overline{\mu}}(\mu)\Lambda^{\mathrm{du},mb}_{q,k}\\
& + \sum_{q=1}^{Q}\sum_{q'=1}^{Q}\sum_{j=1}^{N_{\mathrm{du}}} \Theta^q(\mu)\psi^o_{Nj}(\mu)\Theta^{q'}(\mu)c_{\overline{\mu}}(\mu)\Lambda^{\mathrm{du},am}_{q,j,q',k}\\
& + \sum_{q=1}^{Q}\sum_{q'=1}^{Q}\sum_{j=1}^{N_{\mathrm{du}}}\sum_{j'=1}^{N_{\mathrm{du}}} \Theta^q(\mu)\psi^o_{Nj}(\mu)\Theta^{q'}(\mu)\psi^o_{Nj'}(\mu)\Lambda^{\mathrm{du},aa}_{q,j,q',j',k}\\
& + \sum_{q=1}^{Q}\sum_{q'=1}^{Q} \Theta^q(\mu)\Theta^{q'}(\mu)c^2_{\overline{\mu}}(\mu)\Lambda^{\mathrm{du},mm}_{q,q',k},
\end{aligned}
\tag{A.14}
$$

where the parameter-independent quantities $\Lambda^{\mathrm{du},\cdot}$ are defined as

$$
\begin{aligned}
&\Lambda^{\mathrm{du},bb} = (\hat{z}_0, \hat{z}_0)_X;\\
&\Lambda^{\mathrm{du},ab}_{q,j} = -2(\hat{z}^{\mathrm{du},q}_j, \hat{z}_0)_X \qquad 1 \leqslant q \leqslant Q,\ 1 \leqslant j \leqslant N_{\mathrm{du,max}};\\
&\Lambda^{\mathrm{du},mb}_{q,k} = -2(\hat{x}^q, \hat{z}_0)_X \qquad 1 \leqslant k \leqslant K,\ 1 \leqslant q \leqslant Q;\\
&\Lambda^{\mathrm{du},am}_{q,j,q',k} = 2(\hat{z}^{\mathrm{du},q}_j, \hat{x}^{q'}_k)_X \qquad 1 \leqslant k \leqslant K,\ 1 \leqslant q, q' \leqslant Q,\ 1 \leqslant j \leqslant N_{\mathrm{du,max}};\\
&\Lambda^{\mathrm{du},aa}_{q,j,q',j'} = (\hat{z}^{\mathrm{du},q}_j, \hat{z}^{\mathrm{du},q'}_{j'})_X \qquad 1 \leqslant q, q' \leqslant Q,\ 1 \leqslant j,\ j' \leqslant N_{\mathrm{du,max}};\\
&\Lambda^{\mathrm{du},mm}_{q,q',k} = (\hat{x}^q_k, \hat{x}^{q'}_k)_X \qquad 1 \leqslant k \leqslant K,\ 1 \leqslant q, q' \leqslant Q.
\end{aligned}
\tag{A.15}
$$

(We introduce the superscripts "a", "b" and "m" to distinguish amongst the basis functions related to the reduced basis, the output functional, and the deflation, respectively.)

The offline/online decomposition is now clear. In the *offline* stage we first compute the quantities $\hat{z}_0$, $\hat{z}^{\mathrm{du},q}_j$, and $\hat{x}^q_k$ from (A.13) and then evaluate the $\Lambda^{\mathrm{du},\cdot}$ of (A.15); this requires (to leading order) $\mathrm{O}(Q(N_{\mathrm{du,max}} + K))$ expensive "truth" finite element solutions and $\mathrm{O}(KQ^2N_{\mathrm{du,max}}) + \mathrm{O}(Q^2N^2_{\mathrm{du,max}})$ $\mathcal{N}_{\mathrm{t}}$-inner products. In the *online* stage, given a new parameter value μ and associated reduced basis solutions $u_N(\mu)$ and $\psi_N(\mu)$, the operation count to perform the sum (A.14) is $\mathrm{O}(Q^2(N_{\mathrm{du,max}} + 1)^2)$; the online storage is $\mathrm{O}(KQ^2N_{\mathrm{du,max}}) + \mathrm{O}(Q^2N^2_{\mathrm{du,max}})$.

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