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Numerical Analysis

A successive constraint linear optimization method for lower bounds of parametric coercivity and inf–sup stability constants

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Abstract

We present an approach to the construction of lower bounds for the coercivity and inf–sup stability constants required in a posteriori error analysis of reduced basis approximations to affinely parametrized partial differential equations. The method, based on an Offline–Online strategy relevant in the reduced basis many-query and real-time context, reduces the Online calculation to a small Linear Program: the objective is a parametric expansion of the underlying Rayleigh quotient; the constraints reflect stability information at optimally selected parameter points. Numerical results are presented for coercive elasticity and non-coercive acoustics Helmholtz problems. ***To cite this article: D.B.P. Huynh et al., C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

Résumé

Une méthode d'optimisation linéaire de contraintes successives pour les bornes inférieures des constantes paramétriques de coercivité et de stabilité inf–sup. Nous présentons une méthode pour le calcul de bornes inférieures pour les constantes de stabilité (de coercivité ou d'inf–sup) nécessaires pour les estimateurs d'erreur a posteriori, associées à l'approximation par base réduite d'équations aux dérivées partielles ayant une dépendance affine en les paramétres. La méthode—basée sur une stratégie hors-ligne/en-ligne intéressante pour le calcul temps réel et les cas d'évaluations multiples—réduit le calcul en-ligne à un problème d'optimisation linéaire peu coûteux. La fonction objectif est un développement paramétrique du quotient de Rayleigh. Les contraintes traduisent la stabilité pour un ensemble optimal de paramétres. Nous présentons des résultats numériques pour un problème d'élasticité (coercif) ainsi que pour un problème d'acoustique de type Helmholtz (non-coercif). ***Pour citer cet article : D.B.P. Huynh et al., C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

Version française abrégée

On construit une borne inférieure de la constante de stabilité (de coercivité ou d'inf–sup (2)). La forme bilinéaire a, associée à l'équation aux dérivees partielles posée sur un domaine Ω, dépend de manière affine (voir (1)) d'un

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paramètre $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^P$. On note $X^{\mathcal{N}}(\Omega)$ le sous-espace d'approximation des éléments finis de référence. Ce sous-espace est typiquement de grande dimension $\mathcal{N}$, et il est muni de la norme $\|\cdot\|_{X^{\mathcal{N}}}$ équivalente à la norme $H^1(\Omega)$.

On considère d'abord le cas coercif. On développe le quotient de Rayleigh (2) sous forme paramétrique : $\alpha^{\mathcal{N}}(\boldsymbol{\mu}) = \min_{y\in\mathcal{Y}} \mathcal{J}(\boldsymbol{\mu}; y)$, où $\mathcal{J}(\boldsymbol{\mu}; y) = \sum_{q=1}^{Q} \Theta^q(\boldsymbol{\mu}) y_q$, et l'ensemble $\mathcal{Y}$ est donné par (3). On introduit alors en (4) l'ensemble $\mathcal{Y}_{\mathrm{LB}}$, à partir duquel on construit la borne inférieure (5) comme précisé dans la Proposition 1. La borne inférieure (5) est en fait un problème d'optimisation linéaire de Q variables sous $2Q + M_\alpha + M_+$ contraintes ; M_α et M_+ sont les nombres de contraintes de stabilité et de positivité, respectivement. (Nous introduisons aussi une borne supérieure sur la constante de coercivité servant de critère d'arrêt dans l'étape hors-ligne.)

Nous adoptons une stratégie hors-ligne/en-ligne intéressante dans le cadre d'approximations par la méthode de base réduite en temps réel et pour des évaluations nombreuses. Dans la première étape, hors-ligne, on trouve un ensemble optimal de contraintes de stabilité. Pour obtenir une borne inférieure de précision suffisante pour tout $\boldsymbol{\mu} \in \mathcal{D}$, cette étape (coûteuse) requiert la résolution de $2Q + K_{\max}$ problèmes aux valeurs propres, où $K_{\max}$ est le nombre total de contraintes de stabilité (d'où on tire les M_α plus proches valeurs pour le $\boldsymbol{\mu}$ considéré). Dans la deuxième étape, en-ligne, on calcule la borne inférieure étant donné une valeur $\boldsymbol{\mu} \in \mathcal{D}$ arbitraire. Cette étape requiert la résolution du problème d'optimisation linéaire (5). Le coût de calcul est alors indépendant de $\mathcal{N}$.

Dans le cas non-coercif, on remarque d'abord que $(\beta^{\mathcal{N}}(\boldsymbol{\mu}))^2$ peut s'exprimer comme un problème coercif équivalent, (6). On peut donc faire directement appel à l'approche coercive. Le problème d'optimisation linéaire qui s'ensuit est maintenant posé avec $\widehat{Q} \equiv Q(Q+1)/2$ variables obéissant à $2\widehat{Q} + M_\alpha + M_+$ contraintes.

Nous présentons un exemple d'élasticité linéaire orthotropique (coercif) avec $P = 4$ paramètres pour lequel notre méthode donne $K_{\max} = 50$ pour les choix $M_\alpha = 12$ et $M_+ = 0$. Dans l'étape en-ligne, la borne inférieure $\boldsymbol{\mu} \to \alpha_{\mathrm{LB}}(\boldsymbol{\mu})$ est obtenue cent fois plus vite que pour le calcul direct $\boldsymbol{\mu} \to \alpha^{\mathcal{N}}(\boldsymbol{\mu})$ (même pour ce problème de dimension deux, de taille $\mathcal{N} = 1296$ assez petite).

Nous considérons comme exemple non-coercif un problème d'acoustique de type Helmholtz. Pour minimiser l'effort hors-ligne, on prend $M_\alpha = \infty$ (en fait, en-ligne, $M_\alpha = K_{\max}$) et $M_+ = 4$, ce qui donne $K_{\max} = 22$. Pour minimiser l'effort en-ligne, on prend $M_\alpha = 4$ et $M_+ = 4$, ce qui donne $K_{\max} = 98$. Finalement, pour bien équilibrer les efforts des étapes hors-ligne et en-ligne, on propose $M_\alpha = 16$ et $M_+ = 4$, ce qui donne $K_{\max} = 25$. Dans ce dernier cas, la borne inférieure $\boldsymbol{\mu} \to \beta_{\mathrm{LB}}(\boldsymbol{\mu})$ est obtenue plus de cent fois plus vite que par le calcul direct $\boldsymbol{\mu} \to \beta^{\mathcal{N}}(\boldsymbol{\mu})$. La nouvelle méthode est plus efficace que la technique proposée en [10]. De plus, et c'est sans doute le plus important, elle admet une mise en oeuvre beaucoup plus simple et générale.

1. Introduction

We define the spatial dimension d and the dimension of our field variable d_v; for a scalar field, $d_v = 1$, whereas for a vector field, $d_v = d$. We introduce a regular spatial domain $\Omega \subset \mathbb{R}^d$ with boundary $\partial\Omega$; a typical point in Ω shall be denoted $x = (x_1, \ldots, x_d)$. Finally, we define the 'exact' Hilbert space $X^{\mathrm{e}}(\Omega)$ with inner product $(w, v)_{X^{\mathrm{e}}}$ and induced norm $\|w\|_{X^{\mathrm{e}}} \equiv \sqrt{(w, w)_{X^{\mathrm{e}}}}$. For our class of problems, $(H_0^1(\Omega))^{d_v} \subset X^{\mathrm{e}} \subset (H^1(\Omega))^{d_v}$: $H^1(\Omega) \equiv \{v \in L^2(\Omega) \mid \nabla v \in (L^2(\Omega))^d\}$ with inner product $(w, v)_{H^1} \equiv \int_\Omega \nabla w \cdot \nabla v + wv$ and norm $\|w\|_{H^1} \equiv \sqrt{(w, w)_{H^1}}$; $H_0^1(\Omega) \equiv \{v \in H^1(\Omega) | v|_{\partial\Omega} = 0\}$; and $L^2(\Omega) \equiv \{v \text{ measurable} \mid \int_\Omega v^2 \text{ finite}\}$ with inner product $(w, v)_{L^2} \equiv \int_\Omega wv$ and norm $\|w\|_{L^2} \equiv \sqrt{(w, w)_{L^2}}$. We permit any inner product $(w, v)_{X^{\mathrm{e}}}$ that induces a norm equivalent to the $(H^1(\Omega))^{d_v}$ norm.

We introduce a bounded closed parameter domain $\mathcal{D} \subset \mathbb{R}^d$; we denote a parameter point in $\mathcal{D}$ as $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_P)$. We denote the parametric bilinear form associated with our partial differential equation (PDE) as $a : X^{\mathrm{e}} \times X^{\mathrm{e}} \times \mathcal{D} \to \mathbb{R}$. We define the inf–sup, coercivity, and continuity constants as $\beta^{\mathrm{e}}(\boldsymbol{\mu}) \equiv \inf_{w\in X^{\mathrm{e}}} \sup_{v\in X^{\mathrm{e}}} [a(w, v; \boldsymbol{\mu})/(\|w\|_{X^{\mathrm{e}}} \|v\|_{X^{\mathrm{e}}})]$, $\alpha^{\mathrm{e}}(\boldsymbol{\mu}) \equiv \inf_{w\in X^{\mathrm{e}}} [a(w, w; \boldsymbol{\mu})/(\|w\|^2_{X^{\mathrm{e}}})]$, and $\gamma^{\mathrm{e}}(\boldsymbol{\mu}) \equiv \sup_{w\in X^{\mathrm{e}}} \sup_{v\in X^{\mathrm{e}}} [a(w, v; \boldsymbol{\mu})/(\|w\|_{X^{\mathrm{e}}} \|v\|_{X^{\mathrm{e}}})]$. We assume that a is stable, $\beta^{\mathrm{e}}(\boldsymbol{\mu}) > 0, \forall \boldsymbol{\mu} \in \mathcal{D}$, and continuous, $\gamma^{\mathrm{e}}(\boldsymbol{\mu})$ finite, $\forall \boldsymbol{\mu} \in \mathcal{D}$; if in addition $\alpha^{\mathrm{e}}(\boldsymbol{\mu}) > 0, \forall \boldsymbol{\mu} \in \mathcal{D}$, we say that a is coercive. We assume here that a is symmetric: $a(w, v) = a(v, w), \forall w, v \in X^{\mathrm{e}}$; see [3] for the non-symmetric case. We also introduce a linear bounded functional, $f : X^{\mathrm{e}} \to \mathbb{R}$.

We assume that our bilinear form is 'affine' in the parameter: for some finite small Q,

$$a(w, v; \boldsymbol{\mu}) \equiv \sum_{q=1}^{Q} \Theta^q(\boldsymbol{\mu}) a^q(w, v), \quad \forall w, v \in X^{\mathrm{e}}, \tag{1}$$

where the Θ^q, $1 \leqslant q \leqslant Q$, are continuous functions over $\mathcal{D}$, and the a^q, $1 \leqslant q \leqslant Q$, are symmetric continuous bilinear forms over $X^{\mathrm{e}} \times X^{\mathrm{e}}$. The assumption (1) is crucial in Offline–Online strategies.

Our problem statement is then: given $\boldsymbol{\mu} \in \mathcal{D}$, find $u^{\mathrm{e}}(\boldsymbol{\mu}) \in X^{\mathrm{e}}$ such that $a(u^{\mathrm{e}}(\boldsymbol{\mu}), v; \boldsymbol{\mu}) = f(v), \forall v \in X^{\mathrm{e}}$; then evaluate the output $s^{\mathrm{e}}(\boldsymbol{\mu}) = f(u^{\mathrm{e}}(\boldsymbol{\mu}))$. (In general, we can consider $s(\boldsymbol{\mu}) = \ell(u^{\mathrm{e}}(\boldsymbol{\mu}))$ for bounded $\ell : X^{\mathrm{e}} \to \mathbb{R}$; here we restrict attention to the linear compliant case, $\ell = f$.)

We introduce a finite element 'truth' approximation space of dimension $\mathcal{N}$, $X^{\mathcal{N}} \subset X^{\mathrm{e}}$, with inherited inner product and norm $(w, v)_{X^{\mathcal{N}}} \equiv (w, v)_{X^{\mathrm{e}}}$ and $\|w\|_{X^{\mathcal{N}}} \equiv \|w\|_{X^{\mathrm{e}}}$. We define

$$\beta^{\mathcal{N}}(\boldsymbol{\mu}) \equiv \inf_{w \in X^{\mathcal{N}}} \sup_{v \in X^{\mathcal{N}}} \frac{a(w, v; \boldsymbol{\mu})}{\|w\|_{X^{\mathcal{N}}} \|v\|_{X^{\mathcal{N}}}}, \qquad \alpha^{\mathcal{N}}(\boldsymbol{\mu}) \equiv \inf_{w \in X^{\mathcal{N}}} \frac{a(w, w; \boldsymbol{\mu})}{\|w\|^2_{X^{\mathcal{N}}}}, \tag{2}$$

and $\gamma^{\mathcal{N}}(\boldsymbol{\mu}) \equiv \sup_{w \in X^{\mathcal{N}}} \sup_{v \in X^{\mathcal{N}}} [a(w, v; \boldsymbol{\mu})/(\|w\|_{X^{\mathcal{N}}} \|v\|_{X^{\mathcal{N}}})]$. It immediately follows that $\alpha^{\mathrm{e}}(\boldsymbol{\mu}) \leqslant \alpha^{\mathcal{N}}(\boldsymbol{\mu})$ and $\gamma^{\mathcal{N}}(\boldsymbol{\mu}) \leqslant \gamma^{\mathrm{e}}(\boldsymbol{\mu})$; we *assume* that $\beta^{\mathcal{N}}(\boldsymbol{\mu}) > 0, \forall \boldsymbol{\mu} \in \mathcal{D}$. Our 'truth' FE approximation is then: given $\boldsymbol{\mu} \in \mathcal{D}$, find $u^{\mathcal{N}}(\boldsymbol{\mu}) \in X^{\mathcal{N}}$ such that $a(u^{\mathcal{N}}(\boldsymbol{\mu}), v; \boldsymbol{\mu}) = f(v), \forall v \in X^{\mathcal{N}}$; then evaluate the output $s^{\mathcal{N}}(\boldsymbol{\mu}) = f(u^{\mathcal{N}}(\boldsymbol{\mu}))$. We suppose that, to the desired accuracy, $u^{\mathcal{N}}(\boldsymbol{\mu})$ is indistinguishable from $u^{\mathrm{e}}(\boldsymbol{\mu})$.

Our interest is in reliable real-time and many-query response $\boldsymbol{\mu} \to s^{\mathcal{N}}(\boldsymbol{\mu})$: in the real-time context such as parameter estimation the premium is on reduced *marginal* cost; in the many-query context such as optimization the premium is on reduced *average* cost. We consider reduced basis methods [7,1,9,6]: we develop Galerkin approximations to $u^{\mathcal{N}}$ and $s^{\mathcal{N}}(\boldsymbol{\mu})$, $u_N(\boldsymbol{\mu}) \in W_N \subset X^{\mathcal{N}}$ and $s_N(\boldsymbol{\mu}) = f(u_N(\boldsymbol{\mu}))$, respectively, as well as (i) a rigorous and relatively sharp a posteriori error bound $\Delta^s_N(\boldsymbol{\mu})$ such that $|s^{\mathcal{N}}(\boldsymbol{\mu}) - s_N(\boldsymbol{\mu})| \leqslant \Delta^s_N(\boldsymbol{\mu}), \forall \boldsymbol{\mu} \in \mathcal{D}$, and (ii) an Offline–Online computational strategy such that, in the Online stage, the marginal (and hence also asymptotic average) cost to compute $\boldsymbol{\mu} \to s_N(\boldsymbol{\mu}), \Delta^s_N(\boldsymbol{\mu})$ depends only on N, the dimension of W_N, and Q—and *not* on $\mathcal{N}$.

The error bound $\Delta^s_N(\boldsymbol{\mu})$ takes the form [6] in the coercive case $\|R(\cdot\,; \boldsymbol{\mu})\|^2_{(X^{\mathcal{N}})'}/\alpha_{\mathrm{LB}}(\boldsymbol{\mu})$ and in the non-coercive case $\|R(\cdot\,; \boldsymbol{\mu})\|^2_{(X^{\mathcal{N}})'}/\beta_{\mathrm{LB}}(\boldsymbol{\mu})$, where $R(v; \boldsymbol{\mu}) \equiv f(v) - a(u_N(\boldsymbol{\mu}), v; \boldsymbol{\mu}), \forall v \in X^{\mathcal{N}}$, is the residual, $\|\cdot\|_{(X^{\mathcal{N}})'}$ denotes the dual norm, and $\alpha_{\mathrm{LB}}(\boldsymbol{\mu})$ and $\beta_{\mathrm{LB}}(\boldsymbol{\mu})$ are lower bounds for the coercivity and inf–sup constants. Our focus in this paper is on a new lower bound (Offline–Online) strategy for $\alpha_{\mathrm{LB}}(\boldsymbol{\mu})$ and $\beta_{\mathrm{LB}}(\boldsymbol{\mu})$. Our new approach is more efficient and general than our earlier coercive [9,6] and non-coercive [6,10] proposals; also the new approach is much more easily implemented.

There are many classical techniques for the estimation of smallest eigenvalues or smallest singular values. One class of methods is based on Gershgorin's theorem and variants [5]. A second class of methods is based on eigenfunction/eigenvalue (e.g., Rayleigh Ritz) approximation and subsequent residual evaluation [8,4]. Unfortunately, in neither case can we obtain the rigor, sharpness, and online efficiency we require.

2. Successive Constraints Method (SCM)

We address the coercive case first. By way of preliminaries we define

$$\mathcal{Y} \equiv \left\{ y = (y_1, \ldots, y_Q) \in \mathbb{R}^Q \;\middle|\; \exists w_y \in X^{\mathcal{N}} \text{s.t. } y_q = \frac{a^q(w_y, w_y)}{\|w_y\|^2_{X^{\mathcal{N}}}}, 1 \leqslant q \leqslant Q \right\}. \tag{3}$$

We further define the objective function $\mathcal{J} : \mathcal{D} \times \mathbb{R}^Q \to \mathbb{R}$ as $\mathcal{J}(\boldsymbol{\mu}; y) = \sum_{q=1}^Q \Theta^q(\boldsymbol{\mu}) y_q$. We may then write our coercivity constant as $\alpha^{\mathcal{N}}(\boldsymbol{\mu}) = \min_{y \in \mathcal{Y}} \mathcal{J}(\boldsymbol{\mu}; y)$; we now consider relaxations.

We first define $\sigma^-_q \equiv \inf_{w \in X^{\mathcal{N}}} [a^q(w, w)/(\|w\|^2_{X^{\mathcal{N}}})]$ and $\sigma^+_q \equiv \sup_{w \in X^{\mathcal{N}}} [a^q(w, w)/(\|w\|^2_{X^{\mathcal{N}}})]$, $1 \leqslant q \leqslant Q$, and let $\mathcal{B}_Q \equiv \prod_{q=1}^Q [\sigma^-_q, \sigma^+_q] \in \mathbb{R}^Q$. We also introduce the two parameter sets $\Xi \equiv \{\nu_1 \in \mathcal{D}, \ldots, \nu_J \in \mathcal{D}\}$ and $\mathcal{C}_K \equiv \{\omega_1 \in \mathcal{D}, \ldots, \omega_K \in \mathcal{D}\}$. For any finite-dimensional subset of $\mathcal{D}$, E ($= \Xi$ or $\mathcal{C}_K$), $\mathcal{P}_M(\boldsymbol{\mu}; E)$ shall denote the M points closest to $\boldsymbol{\mu}$ in E (in the Euclidean norm); if $\mathrm{card}(E) \leqslant M$ then we define $\mathcal{P}_M(\boldsymbol{\mu}; E) = E$, and if $M = 0$ we define $\mathcal{P}_M(\boldsymbol{\mu}; E) = \emptyset$.

For given $\mathcal{C}_K$, $M_\alpha \in \mathbb{N}$ (stability constraints), and $M_+ \in \mathbb{N}$ (positivity constraints), we define

$$\mathcal{Y}_{\mathrm{LB}}(\boldsymbol{\mu}; \mathcal{C}_K) \equiv \left\{ y \in \mathcal{B}_Q \;\middle|\; \right.$$

$$\left.\sum_{q=1}^{Q}\Theta^q(\boldsymbol{\mu}')y_q \geqslant \alpha^{\mathcal{N}}(\boldsymbol{\mu}'), \forall \boldsymbol{\mu}' \in \mathcal{P}_{M_\alpha}(\boldsymbol{\mu}; \mathcal{C}_K); \sum_{q=1}^{Q}\Theta^q(\boldsymbol{\mu}')y_q \geqslant 0, \forall \boldsymbol{\mu}' \in \mathcal{P}_{M_+}(\boldsymbol{\mu}; \Xi)\right\}, \tag{4}$$

and $\mathcal{Y}_{\mathrm{UB}}(\mathcal{C}_K) \equiv \{y^\star(\omega_k), 1 \leqslant k \leqslant K\}$ for $y^\star(\boldsymbol{\mu}) \equiv \arg\min_{y\in\mathcal{Y}} \mathcal{J}(\boldsymbol{\mu}; y)$. We next define

$$\alpha_{\mathrm{LB}}(\boldsymbol{\mu}; \mathcal{C}_K) = \min_{y\in\mathcal{Y}_{\mathrm{LB}}(\boldsymbol{\mu};\mathcal{C}_K)} \mathcal{J}(\boldsymbol{\mu}; y) \tag{5}$$

and $\alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K) = \min_{y\in\mathcal{Y}_{\mathrm{UB}}(\mathcal{C}_K)} \mathcal{J}(\boldsymbol{\mu}; y)$. We then obtain

Proposition 1. *For given $\mathcal{C}_K$ (and $M_\alpha \in \mathbb{N}$, $M_+ \in \mathbb{N}$, Ξ), $\alpha_{\mathrm{LB}}(\boldsymbol{\mu}; \mathcal{C}_K) \leqslant \alpha^{\mathcal{N}}(\boldsymbol{\mu}) \leqslant \alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K), \forall \boldsymbol{\mu} \in \mathcal{D}$.*

Proof. For the upper bound, clearly $\mathcal{Y}_{\mathrm{UB}} \subset \mathcal{Y}$; hence, $\alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K) \geqslant \alpha^{\mathcal{N}}(\boldsymbol{\mu})$. For the lower bound, $\mathcal{Y} \subset \mathcal{Y}_{\mathrm{LB}}$: for example (we consider the stability constraints), for any $y \in \mathcal{Y} \Leftrightarrow w_y \in X^{\mathcal{N}}$ (see (3))

$$\sum_{q=1}^{Q}\Theta^q(\boldsymbol{\mu}')y_q = \sum_{q=1}^{Q}\Theta^q(\boldsymbol{\mu}')\frac{a^q(w_y, w_y)}{\|w_y\|^2_{X^{\mathcal{N}}}} \geqslant \inf_{w\in X^{\mathcal{N}}} \sum_{q=1}^{Q}\Theta^q(\boldsymbol{\mu}')\frac{a^q(w, w)}{\|w\|^2_{X^{\mathcal{N}}}} = \alpha(\boldsymbol{\mu}'), \qquad \forall \boldsymbol{\mu}' \in \mathcal{D};$$

a similar argument applies to the positivity constraints. Hence $\alpha^{\mathcal{N}}(\boldsymbol{\mu}) \geqslant \alpha_{\mathrm{LB}}(\boldsymbol{\mu}; \mathcal{C}_K)$. □

We expect that if $\mathcal{C}_K$ is sufficiently large, (i) $y^\star(\boldsymbol{\mu})$ will be sufficiently close to a member of $\mathcal{Y}_{\mathrm{UB}}$ to provide a good upper bound, and (ii) the stability and positivity constraints in $\mathcal{Y}_{\mathrm{LB}}$ will sufficiently restrict y to provide a good lower bound.

We note that (4), (5) is in fact a linear optimization problem or Linear Program (LP). Our LP (5) contains Q design variables ($y = (y_1, \ldots, y_Q)$) and $2Q$ ($y \in \mathcal{B}_Q$) $+ M_\alpha$ (stability) $+ M_+$ (positivity) inequality constraints. The operation count for the Online stage $\boldsymbol{\mu} \to \alpha_{\mathrm{LB}}(\boldsymbol{\mu})$ is *independent* of $\mathcal{N}$.

But first we must determine $\mathcal{C}_K$ and obtain the $\alpha^{\mathcal{N}}(\omega_k)$, $1 \leqslant k \leqslant K$, by an Offline 'greedy' algorithm. We first set $K = 1$ and choose $\mathcal{C}_1 = \{\omega_1\}$ 'arbitrarily'; we also specify M_α, M_+, Ξ, and a tolerance $\epsilon_\alpha \in]0, 1[$. We then set $K = 1$ and perform

While $\max_{\boldsymbol{\mu}\in\Xi}[(\alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K) - \alpha_{\mathrm{LB}}(\boldsymbol{\mu}; \mathcal{C}_K))/\alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K)] > \varepsilon_\alpha$:
$\omega_{K+1} = \arg\max_{\boldsymbol{\mu}\in\Xi}[(\alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K) - \alpha_{\mathrm{LB}}(\boldsymbol{\mu}; \mathcal{C}_K))/\alpha_{\mathrm{UB}}(\boldsymbol{\mu}; \mathcal{C}_K)]$
$\mathcal{C}_{K+1} = \mathcal{C}_K \cup \omega_{K+1}$; $K \leftarrow K + 1$;
end. Set $K_{\max} = K$.

The notable offline computations are (i) $2Q$ eigenproblems to form $\mathcal{B}_Q$, and $K_{\max}$ eigenproblems to obtain $y^\star(\omega_k), \alpha^{\mathcal{N}}(\omega_k)$, $1 \leqslant k \leqslant K_{\max}$ (for a judiciously chosen inner product, the latter can be efficiently calculated by a Lanczos scheme [3]); (ii) $O(\mathcal{N}QK_{\max})$ operations to form $\mathcal{Y}_{\mathrm{UB}}$ (we assume sparsity); and (iii) $JK_{\max}$ LPs of size $O(Q + M_\alpha + M_+)$.

We now consider the non-coercive case. We introduce operators $T^q : X^{\mathcal{N}} \to X^{\mathcal{N}}$ as

$$(T^q w, v)_{X^{\mathcal{N}}} = a^q(w, v), \quad \forall v \in X^{\mathcal{N}},\ 1 \leqslant q \leqslant Q,$$

and $T^{\boldsymbol{\mu}} w \equiv \sum_{q=1}^{Q}\Theta^q(\boldsymbol{\mu})T^q w$. It is then readily demonstrated [10] that

$$\left(\beta^{\mathcal{N}}(\boldsymbol{\mu})\right)^2 = \inf_{w\in X^{\mathcal{N}}}\left[(T^{\boldsymbol{\mu}} w, T^{\boldsymbol{\mu}} w)_{X^{\mathcal{N}}}/\|w\|^2_{X^{\mathcal{N}}}\right],$$

which can be expanded as

$$\left(\beta^{\mathcal{N}}(\boldsymbol{\mu})\right)^2 = \inf_{w\in X^{\mathcal{N}}}\left[\sum_{q'=1}^{Q}\sum_{q''=q'}^{Q}(2 - \delta_{q'q''})\Theta^{q'}(\boldsymbol{\mu})\Theta^{q''}(\boldsymbol{\mu})\left((T^{q'} w, T^{q''} w)_{X^{\mathcal{N}}}/\|w\|^2_{X^{\mathcal{N}}}\right)\right];$$

here $\delta_{q'q''}$ is the Kronecker delta. We now identify

$$\left(\beta^{\mathcal{N}}(\boldsymbol{\mu})\right)^2 \longmapsto \hat{\alpha}^{\mathcal{N}}(\boldsymbol{\mu}),$$
$$(2 - \delta_{q'q''})\Theta^{q'}(\boldsymbol{\mu})\Theta^{q''}(\boldsymbol{\mu}), \quad 1 \leqslant q' \leqslant q'' \leqslant Q \longmapsto \hat{\Theta}^q(\mu), \quad 1 \leqslant q \leqslant \widehat{Q} \equiv Q(Q+1)/2,$$

and

$$(T^{q'}w, T^{q''}v)_{X^{\mathcal{N}}}, \quad 1 \leqslant q' \leqslant q'' \leqslant Q \longmapsto \hat{a}^q(w,v), \quad 1 \leqslant q \leqslant \widehat{Q},$$

and observe that

$$\left(\beta^{\mathcal{N}}(\boldsymbol{\mu})\right)^2 \equiv \hat{\alpha}^{\mathcal{N}}(\boldsymbol{\mu}) \equiv \inf_{w \in X^{\mathcal{N}}} \sum_{q=1}^{\widehat{Q}} \hat{\Theta}^q(\boldsymbol{\mu}) \frac{\hat{a}^q(w,w)}{\|w\|^2_{X^{\mathcal{N}}}}. \tag{6}$$

We may thus directly apply our SCM procedure to (6), however our LP for $(\beta^{\mathcal{N}}(\boldsymbol{\mu}))^2$ now has $\approx Q^2/2$ design variables and $\approx (Q^2 + M_\alpha + M_+)$ inequality constraints.

3. Numerical results

As a coercive example, we consider a linear elastic orthotropic material [2] in two dimensions (plane stress): $d = d_v = 2$. The original domain is a rectangle $]0, L[\times]0, 1[$: we map this domain to a fixed reference domain $\Omega \equiv]0, L_{\text{ref}} = 1[\times]0, 1[$; subsequently L shall appear only in the parameter-dependent coefficient functions. Our function space X^{e} is given by $\{v \in H^1(\Omega) | v|_{\Gamma^D} = 0\}^2$, where Γ^D is the left boundary of Ω; $X^{\mathcal{N}} \subset X^{\text{e}}$ is a linear finite element space of dimension $\mathcal{N} = 1296$.

We consider $P = 4$ parameters: $\mu_1 \equiv E_{x_2}/E_{x_1}$, where E_{x_2} and E_{x_1} are the orthotropic Young's moduli; $\mu_2 \equiv \nu$, the Poisson ratio; $\mu_3 \equiv G/E_{x_1}$, where G is the tangential modulus; and $\mu_4 \equiv L$. The parameter domain is given by

$$\mathcal{D} \equiv [0.05, 1.0] \times [0.1, 0.3225] \times [0.02, 0.50] \times [0.1, 15].$$

Our affine development (1) then applies for $Q = 6$ and

$$\Theta^1(\boldsymbol{\mu}) = \frac{1}{\mu_4(1-\mu_2^2)}, \qquad a^1(v,w) = \int_\Omega \frac{\partial v_1}{\partial x_1}\frac{\partial w_1}{\partial x_1},$$

$$\Theta^2(\boldsymbol{\mu}) = \frac{\mu_2}{1-\mu_2^2}, \qquad a^2(v,w) = \int_\Omega \left(\frac{\partial v_2}{\partial x_2}\frac{\partial w_1}{\partial x_1} + \frac{\partial v_1}{\partial x_1}\frac{\partial w_2}{\partial x_2}\right),$$

$$\Theta^3(\boldsymbol{\mu}) = \mu_3\mu_4, \qquad a^3(v,w) = \int_\Omega \frac{\partial v_1}{\partial x_2}\frac{\partial w_1}{\partial x_2}$$

$$\Theta^4(\boldsymbol{\mu}) = \mu_3, \qquad a^4(v,w) = \int_\Omega \left(\frac{\partial v_1}{\partial x_2}\frac{\partial w_2}{\partial x_1} + \frac{\partial v_2}{\partial x_1}\frac{\partial w_1}{\partial x_2}\right),$$

$$\Theta_5(\boldsymbol{\mu}) = \frac{\mu_3}{\mu_4}, \qquad a^5(v,w) = \int_\Omega \frac{\partial v_2}{\partial x_1}\frac{\partial w_2}{\partial x_1},$$

$$\Theta_6(\boldsymbol{\mu}) = \frac{\mu_1\mu_4}{1-\mu_2^2}, \qquad a^6(v,w) = \int_\Omega \frac{\partial v_2}{\partial x_2}\frac{\partial w_2}{\partial x_2}.$$

We choose for our inner product $(w,v)_{X^{\mathcal{N}}} \equiv a(w, v; \boldsymbol{\mu}_{\text{ref}} = \{1.0, 0.1, 0.5, 1.0\}) + \lambda_{\min}(w,v)_{L^2}$, where $\lambda_{\min}$ is the minimum of the Rayleigh quotient $a(w,w;\boldsymbol{\mu}_{\text{ref}})/(w,w)_{L^2}$; this choice of inner product ensures a good spectrum for the Lanczos algorithm [3].

We apply our greedy algorithm for $\epsilon_\alpha = .75$ and Ξ a random sample of size $J = 1500$. For $M_\alpha = \infty$ (effectively $M_+ = K_{\max}$ in the Online stage) and $M_+ = 0$ we obtain $K_{\max} = 30$. However, we can significantly reduce M_α (and Online effort) with only a slight increase in $K_{\max}$ (and Offline effort): for $M_\alpha = 12$, $M_+ = 0$, we obtain $K_{\max} = 50$. (Note that since $M_+ = 0$, our lower bound is a constructive proof that a is coercive over Ξ.) For this 'optimal' set of parameters, we observe that our Online lower bound $\boldsymbol{\mu} \to \alpha_{\text{LB}}(\boldsymbol{\mu})$ is ≈ 100 times faster than direct computation of $\boldsymbol{\mu} \to \alpha^{\mathcal{N}}(\boldsymbol{\mu})$.

As a non-coercive example, we consider a simple acoustics (microphone probe) Helmholtz problem [10] in two dimensions: $d = 2$, $d_v = 1$. The original domain is a channel probe followed by a microphone plenum of height

$1/4 + L$: we map this domain to a fixed reference domain ($L_{\mathrm{ref}} = 1$) $\overline{\Omega} = [-1/2, 1] \times [0, 1/4] \cup [0, 1] \times [1/4, 5/4]$; subsequently L shall appear only in the parameter-dependent coefficient functions. Our function space X^{e} is given by $\{v \in H^1(\Omega) | v|_{\Gamma^D} = 0\}$ where Γ^D is the left boundary of Ω; $X^{\mathcal{N}} \subset X^{\mathrm{e}}$ is then a quadratic finite element space of dimension $\mathcal{N} = 4841$ over a triangulation of Ω.

We consider $P = 2$ parameters: $\mu_1 \equiv L$, and $\mu_2 = k^2$ (the reduced frequency squared); the parameter domain $\mathcal{D} \equiv [0.3, 0.6] \times [3.0, 6.0]$ lies between the first and second resonances. Our affine development (1) then applies [10] for $Q = 5$ and hence $\widehat{Q} = Q(Q + 1)/2 = 15$. For our inner product we choose $(w, v)_{X^{\mathcal{N}}} \equiv a_0(w, v) + \lambda_{\min}(w, v)_{L^2}$, where $a_0(w, v) \equiv a(w, v; (0.45, 0))$ and $\lambda_{\min}$ is the minimum of the Rayleigh quotient $a_0(w, w)/(w, w)_{L^2}$.

We apply our greedy algorithm for $\epsilon_\alpha = 0.75$ and Ξ a random sample of size $J = 3671$. For the case $M_\alpha = \infty$ (effectively, $M_\alpha = K_{\max}$ in the Online stage) and $M_+ = 4$ we obtain $K_{\max} = 22$: this choice minimizes the Offline effort. If we wish to minimize the Online effort we can choose $M_\alpha = 4$ (and $M_+ = 4$)—note the Online effort is independent of $K_{\max}$—which then yields $K_{\max} = 98$: in this case, our Online lower bound $\boldsymbol{\mu} \to \beta_{\mathrm{LB}}(\boldsymbol{\mu})$ is ≈ 160 times faster than direct computation of $\boldsymbol{\mu} \to \beta^{\mathcal{N}}(\boldsymbol{\mu})$. For a better Offline–Online balance we can consider $M_\alpha = 16$, $M_+ = 4$ which yields $K_{\max} = 25$: in this case, our Online lower bound $\boldsymbol{\mu} \to \beta_{\mathrm{LB}}(\boldsymbol{\mu})$ is ≈ 137 times faster than direct computation of $\boldsymbol{\mu} \to \beta^{\mathcal{N}}(\boldsymbol{\mu})$. We have also applied the SCM approach to the (in fact, coercive) parameter domain considered in [10]; the SCM performs better than the natural norm approach of [10], and is also much simpler to implement.

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