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A successive constraint method with minimal offline constraints for lower bounds of parametric coercivity constant. Une méthode par contraintes successives avec un minimum de contraintes hors ligne pour les bornes inférieures des constantes de coercivité à dépendance paramétrique.

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Abstract

A posteriori error estimates are a key ingredient for the certified reduced basis method. Sharp error bounds rely on the construction of lower bounds for the coercivity or inf-sup stability constant. The Successive Constraint Method (SCM) has been previously proposed to compute such lower bounds, using an efficient Offline-Online strategy. We present in this article some modifications to the SCM to get rid of user-dependent parameters, which also improve convergence and reduce the computational cost of the method.

Les estimateurs d'erreur a posteriori sont un élément clé de la méthode des bases réduites certifiées. L'obtention d'estimateurs précis repose sur la construction de bornes inférieures pour la constante de coercivité ou de stabilité inf-sup. La Méthode par Contraintes Successives (SCM) a été proposée afin de calculer de telles bornes inférieures, en utilisant une stratégie efficace hors ligne-en ligne. Dans cet article, nous présentons certaines modifications à la SCM afin de se passer de paramètres dépendant de l'utilisateur. Ces modifications permettent également d'avoir une convergence plus rapide de la méthode, ainsi qu'un gain computationnel significatif.

Keywords: Reduced basis method, Successive constraint method, Méthode bases réduites, Méthode par contraintes successives

1. Successive constraint method

This section describes the Successive Constraint Method (SCM) as first introduced in [1] and then improved in [2].

Starting from an affine bilinear form

$$a(w, v; \mu) = \sum_{q=1}^Q \theta_q(\mu) a_q(w, v), \quad w, v \in X^N, \quad \mu \in \mathcal{D}$$

we wish to compute $\alpha^{\text{LB}} : \mathcal{D} \rightarrow \mathbb{R}$ such that $0 < \alpha^{\text{LB}}(\mu) \leq \alpha^N(\mu)$, $\mu \in \mathcal{D}$ where $\alpha^N(\mu)$ is the coercivity constant

$$\alpha^N(\mu) = \inf_{w \in X^N} \frac{a(w, w; \mu)}{\|w\|_X^2}$$

Hence we have that

$$\alpha^N(\mu) = \inf_{y \in \mathcal{Y}} \mathcal{J}^{\text{obj}}(\mu; y) \quad \text{where} \quad \mathcal{J}^{\text{obj}}(\mu; y) \equiv \sum_{q=1}^Q \theta_q(\mu) y_q$$
$$\mathcal{Y} = \left\{ y \in \mathbb{R}^Q \mid \exists w \in X^N \text{ s.t. } y_q = \frac{a_q(w, w)}{\|w\|_X^2}, 1 \leq q \leq Q \right\} \quad (1)$$

We now need to characterize \mathcal{Y} , to do this we construct two sets \mathcal{Y}_{LB} and \mathcal{Y}_{UB} such that $\mathcal{Y}_{\text{UB}} \subset \mathcal{Y} \subset \mathcal{Y}_{\text{LB}}$ over which (1) is feasible. First we set the design space for the minimisation problem (1). We introduce

$$\mathcal{B} = \prod_{q=1}^Q \left[\inf_{w \in \mathcal{X}^N} \frac{a_q(w, w)}{\|w\|_{\mathcal{X}}^2}; \sup_{w \in \mathcal{X}^N} \frac{a_q(w, w)}{\|w\|_{\mathcal{X}}^2} \right]$$

$$\Xi = \left\{ \mu_i \in \mathcal{D}; i = 1, \dots, J \right\} \quad \text{and} \quad C_K = \left\{ \mu_i \in \Xi; i = 1, \dots, K \right\} \subset \Xi$$

Ξ is a fine sampling of \mathcal{D} . C_K will be constructed using a greedy algorithm. Finally we denote $P_M(v; E)$ the set of M points closest to v in the set E .

1.1. Lower bounds

Given $M_\alpha, M_+ \in \mathbb{N}$ we are now ready to define \mathcal{Y}_{LB} and α_{LB}

$$\mathcal{Y}_{\text{LB}}(v; C_K) = \left\{ y \in \mathcal{B} \mid \sum_{q=1}^Q \theta_q(v') y_q \geq \alpha^N(v'), \forall v' \in P_{M_\alpha}(v; C_K) \right. \\ \left. \sum_{q=1}^Q \theta_q(v') y_q \geq \alpha_{\text{LB}}(v'; C_{K-1}), \forall v' \in P_{M_+}(v; \Xi \setminus C_K) \right\} \quad (2)$$

$$\alpha_{\text{LB}}(v; C_K) = \inf_{y \in \mathcal{Y}_{\text{LB}}(v; C_K)} \mathcal{J}^{\text{obj}}(v; y) \quad (3)$$

(3) is in fact a linear program with Q design variables, y_q , and $2Q + M_\alpha + M_+$ constraints online. It requires the construction of C_K offline.

1.2. Upper bounds

$$\mathcal{Y}_{\text{UB}}(C_K) = \left\{ y^*(\mu_k), 1 \leq k \leq K \right\} \quad \text{with} \quad y^*(v) = \operatorname{argmin}_{y \in \mathcal{Y}} \mathcal{J}^{\text{obj}}(v; y)$$

$$\alpha_{\text{UB}}(v; C_K) = \inf_{y \in \mathcal{Y}_{\text{UB}}(C_K)} \mathcal{J}^{\text{obj}}(v; y) \quad (4)$$

\mathcal{Y}_{UB} requires K eigensolves to compute the eigenmode η_k associated with $w_k, k = 1, \dots, K$ and KQN inner products to compute the $y_q^*(w_k) = \frac{a_q(\eta_k, \eta_k)}{\|\eta_k\|_{\mathcal{X}^N}^2}, k = 1, \dots, K$ offline. Then (4) is a simple enumeration online.

1.3. Construction of C_K

Given Ξ and $\epsilon \in [0; 1]$

While $\max_{v \in \Xi} \frac{\alpha_{\text{UB}}(v; C_K) - \alpha_{\text{LB}}(v; C_K)}{\alpha_{\text{UB}}(v; C_K)} > \epsilon$

- $\mu_{K+1} = \operatorname{argmax}_{v \in \Xi} \frac{\alpha_{\text{UB}}(v; C_K) - \alpha_{\text{LB}}(v; C_K)}{\alpha_{\text{UB}}(v; C_K)}$
- $C_{K+1} = C_K \cup \{\mu_{K+1}\}, K \leftarrow K + 1$

2. Discarding M_α and M_+

For the computation of the lower bound, the two parameters M_α and M_+ must be set by the user, who is supposed to have at least a basic knowledge of the SCM and what these parameters are meant to be. This is quite disappointing as the SCM is part of a framework for reduced basis a posteriori error computation, which should be usable like a black box. Moreover, even for someone familiar with the SCM, it is not straightforward to tune these parameters. Thus we propose a modification of the SCM which does not need the parameters M_α and M_+ , and gives a faster convergence.

2.1. Offline construction of C_K

The constraints of the LP (2) for a given v are basically corresponding to the definition of the coercivity constant taken at neighboring points v' of v . For some of the first kind, the actual coercivity constant has been computed, ($v' \in P_{M_\alpha}(v; C_K)$), for others of the second kind, only a lower bound is available ($v' \in P_{M_+}(v; \Xi \setminus C_K)$). Actually, when building the C_K spaces, the lower bound estimates are rather poor, at least for the first iterations. So the constraints of the second kind are not as good as the constraints of the first kind. Therefore, the first idea is to completely drop M_+ and to keep only the constraint of the second kind for $v' = v$, which enforces the monotonic decreasing of the stopping criterion. The next idea to get rid of M_α is to keep in mind that in a LP with Q variables, there are at most Q active constraints when the minimum is reached. It is also straightforward to see that among all constraints of the first kind, if a constraint is not active at rank K , it will not be active for all ranks $J \geq K$. So while building the C_K spaces, we can keep track of these active constraints (of the first kind), which is easy because there is only to look if the new constraint given by μ_K is active. So we never get more than Q constraints of the first kind, therefore M_α is not needed anymore. One can note that there is no guarantee that the active constraints correspond to the neighboring points $v' \in P_{M_\alpha}(v; C_K)$. As a consequence, taking the active constraints instead of the neighboring constraints will give at least the same results, but more likely better results. Moreover, computing neighbors can be expensive if the trial sampling is big, this problem vanishes when considering the active constraints. To make things clear, with these modifications the space \mathcal{Y}_{LB} at iteration K now reads :

$$\mathcal{Y}_{LB}(v; C_K) = \left\{ y \in \mathcal{B} \mid \begin{array}{l} \sum_{q=1}^Q \theta_q(v') y_q \geq \alpha^N(v'), \quad \forall v' \in A(v; C_{K-1}) \\ \sum_{q=1}^Q \theta_q(\mu_K) y_q \geq \alpha^N(\mu_K) \end{array} \right\}$$

where $A(v; C_{K-1})$ denotes the set of active constraints at minimum for the computation of $\alpha_{LB}(v; C_{K-1})$. After $\alpha_{LB}(v; C_K)$ is computed, we check which constraints are active among $A(v; C_{K-1}) \cup \mu_K$ and store the active ones in $A(v; C_K)$.

2.2. Online computation of α_{LB}

For the online computation of $\alpha_{LB}(v)$, we start from the same idea : the best constraints are from the first kind, and only a few are active. But in this case, we have to deal with $v \notin \Xi$, so the active set of constraints has not been built during the construction of C_K . So to be sure to have the best constraints, one can use all the $\mu_k \in C_K$. This is a rather brute force approach, but the computation is not so expensive as it corresponds to a linear program with few variables and many constraints, so it can be solved very rapidly by considering the dual problem.

3. A short example

We illustrate our modifications on a simple 2D steady-state diffusion equation $\nabla \cdot (k \nabla u) = 0$, in a square domain where k is piecewise constant as described in figure 1 (the thermal block problem [3]). The $k_i, i = 1..9$ are the parameters of the PDE. One shall note that the problem is parametrically coercive, which means that in the affine decomposition

$$\forall \mu \in \mathcal{D}, \theta_q(\mu) > 0 \quad \text{and} \quad \forall w \in X^N, a_q(w, w) \geq 0 \quad 1 \leq q \leq Q.$$

So in this case, a lower bound for the coercivity constant can easily be computed without the need of the SCM [3]. We still consider the thermal block as a toy example to show the advantage of our proposed modifications.

We show in figure 2 the value of the stopping criterion $\frac{\alpha_{UB} - \alpha_{LB}}{\alpha_{UB}}$ with respect to K during the construction of the C_K spaces (with $Card(\Xi) = 10000$). With the proposed modifications, there are at most 10 constraints in the linear programs, yet we get a better convergence rate to what is obtained with the former SCM with $M_\alpha = 10$ and $M_+ = 10$, i.e. with 20 constraints. It underlines the fact that the best constraints are not necessarily given by the neighboring points. Moreover, because we avoid neighbors, there is a significant gain in computational cost : reaching $K = 300$ takes 8h for the SCM with neighbors, but only 9mn for the proposed SCM. Also, we used a kd-tree structure to compute the neighbors efficiently, but it is very

memory demanding, that is why the red curve in figure 2 stops at $K = 300$. Such a problem is completely avoided with the proposed SCM.

As described above, our modifications could be a drawback for online computation, because in this case taking the best constraints means taking all the constraints from C_K , i.e. K constraints. On this example, for $K = 1500$, it took $1mn$ to compute online 10^5 different lower bounds, so it does not appear to be much of a problem.

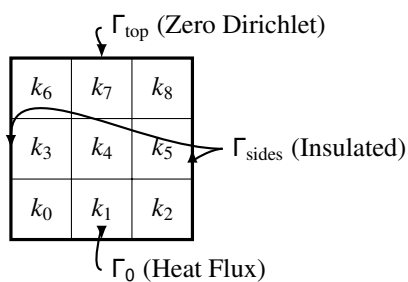


Figure 1: Domain geometry. Géométrie du domaine.

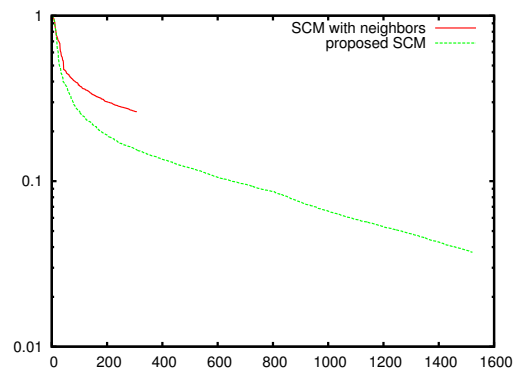


Figure 2: Value of the stopping criterion with respect to K . Valeur du critère d'arrêt en fonction de K .

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