Optimal greedy parameter selection in the reduced basis context

Amina Benaceur

January 17, 2025

1 Basic notation

Let us also introduce a continuous linear form $f : X \to \mathbb{R}$ and a family of symmetric continuous bilinear forms $a : X \times X \times \mathcal{P} \to \mathbb{R}$. We assume that a is symmetric, i.e. $a(v, w; \mu) = a(w, v; \mu)$, $\forall w, v \in X$, $\forall \mu \in D$; and coercive: $\exists \alpha_0 > 0, \forall \mu \in D, \alpha_0 \leq \alpha(\mu) = \inf_{w \in X} \frac{a(w,w;\mu)}{\|w\|_X^2}$. In all that follows, $< \cdot, \cdot >$ denotes a suitable inner product, for instance that of $L^2(\Omega)$ and $\| \cdot \|_X$ is the corresponding norm. Consider the elliptic parameter-dependent problem: find $u(\mu) \in X$ s.t.

$$a(u(\mu), w; \mu) = f(w), \quad \forall w \in X. \tag{1}$$

The reduced basis method has been introduced for the sake of addressing such parameter-dependent problems.

A key purpose is to select the best parameters that would lead to an optimal reduced order model.

2 The strong greedy algorithm

Let $\mathcal{H}$ be a Hilbert space of real-valued functions defined on a spatial domain $\Omega \subset \mathbb{R}^d$, where $d \in \mathbb{N}^*$, and let $\mathcal{K} \subset \mathcal{H}$ be a compact set. The Hilbert space $\mathcal{H}$ is endowed with an inner product $(\cdot, \cdot)$ and a norm $\| \cdot \|$. For a subspace $X \subset \mathcal{H}$, we introduce the projector Π_X onto X. Finally, we consider a discrete training parameter set $\mathcal{P}^{\text{tr}} \subset \mathcal{P}$. Greedy algorithms have been widely investigated in the literature to select parameter values. Their main purpose is seeking a collection of functions $\{u(\mu_1), \ldots, u(\mu_n)\}$ that produces accurate approximations of all functions $f \in \mathcal{P}$. The key idea of the greedy algorithm is to create a set of hierarchical spaces $X_1 \subset X_2 \subset \cdots \subset X_n \subset \cdots \subset \mathcal{K}$, with $\dim(X_n) = n$, that are progressively enriched by a function $h \in \mathcal{K}^{\text{tr}}$ that maximizes a given error.

To start with, we select a function

$$h_1 = \max_{h \in \mathcal{K}^{\text{tr}}} \|h\|, \tag{2}$$

and we define the first approximation space

$$X_1 = \text{span}\{h_1\}. \tag{3}$$

The following approximation spaces are defined by induction. At each new iteration $n > 1$, we select the worst approximated function in X_{n-1}, i.e.

$$h_n = \max_{h \in \mathcal{K}^{\mathrm{tr}}} \|h - \Pi_{X_{n-1}} h\|, \tag{4}$$

and we define the new approximation space

$$X_n = X_{n-1} + \mathrm{span}\{h_n\}. \tag{5}$$

The greedy algorithm is summarized in Algorithm 1.

Algorithm 1 Greedy algorithm

Input : $\mathcal{P}^{\mathrm{tr}}$: training set
ϵ : threshold

```
Search μ_1 = max_{μ ∈ P^tr} ||u(μ)||
Set X_1 = span{u(μ_1)}
while  > ε do
    Search μ_{n+1} = max_{h ∈ P^tr} ||u(μ) − Π_{X_{n−1}} u(μ)||
    Set X_{n+1} = X_n + span{u(μ_{n+1})}
end while
```

Search $\mu_1 = \max_{\mu \in \mathcal{P}^{\mathrm{tr}}} \|u(\mu)\|$
Set $X_1 = \mathrm{span}\{u(\mu_1)\}$
while $> \epsilon$ **do**
  Search $\mu_{n+1} = \max_{h \in \mathcal{P}^{\mathrm{tr}}} \|u(\mu) - \Pi_{X_{n-1}} u(\mu)\|$
  Set $X_{n+1} = X_n + \mathrm{span}\{u(\mu_{n+1})\}$
end while

Output : X_N : reduced space
N : dimension of the final space

We emphasize that the sequence of selected functions $(h_1, \ldots, h_N)$ is not unique thereby implying the non-uniqueness of the error sequence $(e_1, \ldots, e_N)$, where $e_n = \max_{h \in \mathcal{K}^{\mathrm{tr}}} \|h - \Pi_{X_{n-1}} h\|$, for $n \in \{1, \ldots, N\}$.

3 Towards selection uniqueness

The goal of this section is to ensure the uniqueness of the selection resulting from the greedy algorithm. Given a reduced subspace X_{n-1}, assume that

$$\exists\ h_n^1, \ldots, h_n^I \in \mathcal{K}^{\mathrm{tr}} :\ h_n^1, \ldots, h_n^I \in \operatorname*{argmax}_{h \in \mathcal{K}^{\mathrm{tr}}} \|h - \Pi_{X_{n-1}} h\|, \tag{6}$$

for an integer $I \geq 2$. In the standard setting where the choice among $h_n^1, \ldots, h_n^I$ is made randomly, the sequence of errors $(e_1, \ldots, e_N)$ will differ accordingly. In view of a fast decay of the sequence of errors, we suggest to decide on the selection based on the following criterion

$$h_n^i \in \operatorname*{argmin}_{1 \leq i \leq I} \max_{h \in \mathcal{K}^{\mathrm{tr}}} \|h - \Pi_{X_{n-1} + \mathrm{span}\{h_n^1\}} h\| \tag{7}$$

4 Predictive greedy algorithm

The elements that span a reduced space in the reduced basis method are usually selected by means of standard greedy algorithms [1, 2]. The selection strategy that is commonly proposed in the literature is that of enriching the current space with the vector corresponding to the worst approximated parameter, i.e.

$$\mu_{n+1} = \underset{\mu \in \mathcal{P}}{\operatorname{argmax}} \|u(\mu) - P_N u(\mu)\|_X \tag{8}$$

where P_N is the orthogonal projection onto the current reduced subspace $X_N \subset X$. Nevertheless, were we to seek an optimal selection among the available vectors, the criterion would be different. Given a parameter value $\mu \in \mathcal{P}$ and a linear subspace X_N of dimension N, we introduce the linear subspace X^{μ}_{n+1} of dimension $n+1$ defined as follows

$$\begin{aligned} X^{\mu}_{n+1} &= X_N + \operatorname{span}\{u(\mu)\} \\ &= X_N + \operatorname{span}\{\theta_{n+1}(\mu)\} \end{aligned}$$

with

$$\theta_{n+1}(\mu) = \frac{1}{\|u(\mu) - P_N u(\mu)\|_X}\big(u(\mu) - P_N u(\mu)\big).$$

Additionally, we introduce the operator P^{μ}_{n+1} as the orthogonal projection on the subspace X^{μ}_{n+1}.

Proposition 1. *Given a linear subspace $X_N \subset X$, the optimal greedy parameter selection within the discrete parameter set $\mathcal{P}^{\mathrm{tr}}$ at stage $n+1$ is given by*

$$\mu_{n+1} \in \underset{\mu \in \mathcal{P}^{\mathrm{tr}}}{\operatorname{argmin}} \sup_{\nu \in \mathcal{P}^{\mathrm{tr}}} \|u(\nu) - P^{\mu}_{n+1} u(\nu)\|_X \tag{9}$$

Proof. By construction, it holds that

$$\forall \eta \in \mathcal{P}^{\mathrm{tr}}, \qquad \sup_{\nu \in \mathcal{P}^{\mathrm{tr}}} \|u(\nu) - P^{\mu_{n+1}}_{n+1} u(\nu)\|_X \leq \sup_{\nu \in \mathcal{P}^{\mathrm{tr}}} \|u(\nu) - P^{\eta}_{n+1} u(\nu)\|_X.$$

□

The resulting linear subspaces $X_1, \ldots, X_N$ are optimal considering a selection that is restricted to the discrete training parameter space $\mathcal{P}^{\mathrm{tr}}$. We emphasize that they are not optimal in the sense of the Kolmogorov N-width: here, optimality is defined among all the linear N-dimensional subspaces of X that can be spanned by available elements of the solution manifold associated to (1).

Remark 1. *We present a simple example illustrating the suboptimality of the standard greedy criterion* (8)*. Consider $\mathbb{R}^3$ endowed with its canonical scalar product and a solution manifold $\mathcal{M} = \{e_1 = (1,0,0),\ e_2 = (0, 1+\epsilon, 0),\ e_3 = (0,0,1-\epsilon),\ e_4 = \sqrt{2}^{-1}(0,1,1)\}$ with $\epsilon \in [0, 3-2\sqrt{2}[$. Let $X_1 = \operatorname{span}\{e_1\}$ be an initial reduced basis space. The strong greedy algorithm enriches X_1 using e_2 through $X_2 = X_1 + \operatorname{span}\{e_2\}$, leading to $\operatorname{dist}(X_2, \mathcal{M}) = 1 - \epsilon$. Nonetheless, opting for $\tilde{X}_2 = X_1 + \operatorname{span}\{e_4\}$ produces a better reduced basis approximation since it yields $\operatorname{dist}(\tilde{X}_2, \mathcal{M}) = \sqrt{2}^{-1}(1+\epsilon)$.*

Proposition 2. *The optimal greedy selection criterion* (9) *is equivalent to*

$$\mu_{n+1} \in \underset{\mu \in \mathcal{P}^{\mathrm{tr}}}{\operatorname{argmin}} \sup_{\nu \in \mathcal{P}^{\mathrm{tr}}} \left(\|e_n(\nu)\|^2_X - \frac{< e_n(\nu), e_n(\mu) >^2}{\|e_n(\mu)\|^2_X} \right) \tag{10}$$

Proof. A direct expansion of the error norm appearing in (9) gives

$$\begin{aligned}\|u(\nu) - P^{\mu}_{n+1}u(\nu)\|^2_X &= \|u(\nu) - P_N u(\nu) - < u(\nu), \theta_{n+1}(\mu) > \theta_{n+1}(\mu)\|^2_X \\ &= \|u(\nu) - P_N u(\nu)\|^2_X + < u(\nu), \theta_{n+1}(\mu) >^2 \\ &\quad - 2 < u(\nu), \theta_{n+1}(\mu) >< u(\nu) - P_N u(\nu), \theta_{n+1}(\mu) >\end{aligned}$$

Henceforth, we set $e_N(\nu) = u(\nu) - P_N u(\nu)$, for all $\nu \in \mathcal{P}$. Besides, notice that

$$< u(\nu), \theta_{N+1}(\mu) > = < e_n(\nu), \theta_{n+1}(\mu) > . \tag{11}$$

This latter equality (11) implies:

$$\|u(\nu) - P^{\mu}_{N+1}u(\nu)\|_X = \|e_n(\nu)\|^2_X - \frac{1}{\|e_n(\mu)\|^2_X} < e_n(\nu), e_n(\mu) >^2 \tag{12}$$

Consequently, the optimal choice of the parameter μ_{N+1} resulting from (9) is

$$\mu_{N+1} \in \underset{\mu \in \mathcal{P}^{\mathrm{tr}}}{\mathrm{argmin}} \sup_{\nu \in \mathcal{P}^{\mathrm{tr}}} \left(\|e_n(\nu)\|^2_X - \frac{< e_n(\nu), e_n(\mu) >^2}{\|e_n(\mu)\|^2_X} \right)$$

□

Algorithm 2 Predictive greedy algorithm

Input : $\mathcal{P}^{\mathrm{tr}}$: training set
ϵ : threshold

Search $\mu_1 = \underset{\mu \in \mathcal{P}^{\mathrm{tr}}}{\mathrm{argmax}} \|u(\mu)\|$
Set $X_1 = \mathrm{span}\{u(\mu_1)\}$
while $> \epsilon$ **do**
    Search $\mu_{N+1} \in \underset{\mu \in \mathcal{P}^{\mathrm{tr}}}{\mathrm{argmin}} \sup_{\nu \in \mathcal{P}^{\mathrm{tr}}} \left(\|e_n(\nu)\|^2_X - < e_n(\nu), e_n(\mu) >^2 / \|e_n(\mu)\|^2_X \right)$
    Set $X_{n+1} = X_n + \mathrm{span}\{\mu_{n+1}\}$
end while

Output : X_N : reduced space
N : dimension of the final space

5 Ideas

1. Prove that the criterion is decreasing.
2. Look-ahead reduced set of parameters, implying a complexity $N \times M$ instead of N^2.
3. Second reduction step after we've done the first step using the strong greedy algorithm. It implies a squeezing of the basis and possibly spares some vectors.
4. Implement some non-coercive cases where the impact would be even more beneficial.

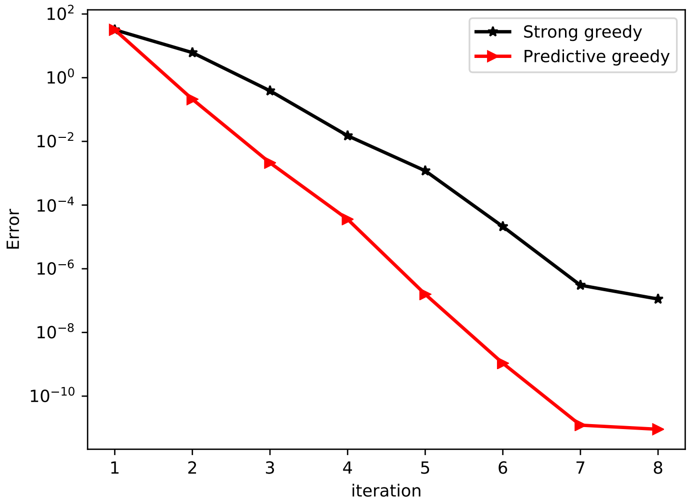

Figure 1: Evaluation of the error $e_n(\mu) = \max_{\mu \in \mathcal{P}^{\mathrm{tr}}} \|u(\mu) - P_{X_n} u(\mu)\|_{\ell^\infty(\Omega^{\mathrm{tr}})}$.

5. The projection error can be replaced by the RB error $\hat{u}(\mu) - u(\mu)$.
6. Ensure the uniqueness of the hierarchical spaces resulting from the greedy algorithm using the predictive criterion.
7. A posteriori reordering of the reduced basis
8. Next step will be to do the same for the CPG algorithm.

6 Numerical results

This section aims at testing the performances of the predictive greedy algorithm compared to the strong greedy algorithm. Let $\mathcal{P} = [0, 20]$ be a parameter set and $\mathcal{P}^{\mathrm{tr}} = \{i | 0 \leq i \leq 20\}$ a chosen training set. We consider a spatial domain $\Omega \in \mathbb{R}^2$, of height $H = 2$m in y and length $L = 4$m in x. We build our training solution manifold using the partial differential equation $0.1\mu\Delta u(\mu) + \sqrt{\mu} u(\mu) = 1$, with homogeneous Neumann boundary conditions on $y = 0$ and $x = 0$, and Dirichlet boundary conditions $u(\cdot, H) = u(L, \cdot) = 1$. We perform both the strong greedy algorithm and the predictive algorithm whose accuracy is displayed in Figure 1.

References

[1] A. Buffa, Y. Maday, A. T. Patera, C. Prud'homme, and G. Turinici. *A priori* convergence of the greedy algorithm for the parametrized reduced basis method. *ESAIM Math. Model. Numer. Anal.*, 46(3):595–603, 2012.

[2] B. Haasdonk. Convergence rates of the POD-greedy method. *ESAIM Math. Model. Numer. Anal.*, 47(3):859–873, 2013.