Méthode des bases réduites probabiliste pour des problèmes paramétrés

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Main problem and objective

We consider the approximation of a family of parameter-dependent functions

$$\mathcal{M} = \{u(\xi) : \xi \in \Xi\}$$

with $\Xi \subset \mathbb{R}^p$ a compact set, and $u(\xi) \in V$ some high-dimensional Hilbert space.

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RBM using pointwise (noisy) evaluations of $u(\xi)$ and in probabilistic setting.

1. Reduced basis greedy algorithm

2. Probabilistic greedy algorithm

3. Application 1 :
Parameter-dependent functions

4. Application 2 :
Parameter-dependent PDEs with probabilistic interpretation

5. Conclusion

Benchmark problem

A benchmark for optimal linear approximation is given by the Kolmogorov n-width

$$d_n(\mathcal{M})_V := \inf_{\dim V_n = n} \sup_{u \in \mathcal{M}} \|u - P_{V_n} u\|_V,$$

where P_{V_n} is the orthogonal projection onto V_n and $\|\cdot\|_V$ is a suitable norm on V.

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- ✗ An optimal space V_n is out of reach, instead **greedy** construction is used.
- ✓ Sequence of nested spaces $\{V_n\}_{n\geq 0}$ obtained from **snapshots** of $u(\xi)$ computed for suitably selected parameter values in Ξ.

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Algorithm 1 : Ideal greedy algorithm

Starting from $V_0 = \{0\}$. Given $\{\xi_1, \dots, \xi_{n-1}\} \subset \Xi$ and the corresponding subspace

$$V_{n-1} = \text{span}\{u(\xi_1), \dots, u(\xi_{n-1})\},$$

a new parameter value ξ_n is selected as

$$\|u(\xi_n) - u_{n-1}(\xi_n)\|_V = \sup_{\xi \in \Xi} \|u(\xi) - u_{n-1}(\xi)\|_V. \tag{1}$$

This ideal algorithm is still unfeasible :

1) the error $\|u(\xi) - u_{n-1}(\xi)\|_V$ for all $\xi \in \Xi$ is not always accessible,
2) maximizing this error over Ξ is a non trivial optimization problem.

Offline : greedy construction of V_n.

Algorithm 1 : Deterministic greedy algorithm

Let $\tilde{\Xi} \subset \Xi$ be a discrete training set and $V_0 = \{0\}$. For $n \geq 1$ proceed as follows.

1) Select
$$\xi_n \in \arg\max_{\xi \in \tilde{\Xi}} \Delta(u_{n-1}(\xi), \xi).$$

2) Compute $u(\xi_n)$ and update $V_n = \text{span}\{u(\xi_1), \dots, u(\xi_n)\}$.

$\Delta(u_n(\xi), \xi)$ is a a suitable error estimate computable from $u_n(\xi)$.

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Online : computation of $u_n(\xi)$.

During the online stage, $u_n(\xi)$ is computed as some projection in V_n with low complexity (depending only on n).

Does it worth it ?

1) If $u_n(\xi)$ is a quasi-optimal projection of $u(\xi)$ onto V_n i.e.

$$\|u(\xi) - u_n(\xi)\|_V \leq C\|u(\xi) - P_{V_n}u(\xi)\|_V \tag{2}$$

for some constant C independent from V_n and ξ.

If $\Delta(u_n(\xi), \xi)$ is certified i.e. there are two constants $0 < m \leq M$ s.t.

$$m\|u(\xi) - u_n(\xi)\|_V \leq \Delta(u_n(\xi), \xi) \leq M\|u(\xi) - u_n(\xi)\|_V. \tag{3}$$

Assuming (2)-(3), there exists $\gamma \in (0, 1]$ such that

$$\|u(\xi_n) - P_{V_{n-1}}u(\xi_n)\|_V \geq \gamma \sup_{\xi\in\Xi} \|u(\xi) - P_{V_{n-1}}u(\xi)\|_V. \tag{4}$$

i.e. the algorithm is a weak-greedy algorithm.

$\rightsquigarrow V_n$ is not optimal but the approximation error

$$\sigma_n(\mathcal{M})_V := \sup_{u\in\mathcal{M}} \|u - P_{V_n}u\|_V$$

decays like $d_n(\mathcal{M})_V$ for algebraic or exponential convergence.
(Binev-Cohen-Dahmen-DeVore-Petrova-Wojtaszczyk,2011), (Buffa-Maday-Patera-Prud'homme-Turinici,2012), (DeVore-Petrova-Wojtaszczyk,2013).

2) Replacing Ξ by $\tilde{\Xi}$ a (finite subset) e.g. ε-net of Ξ (Cohen-Dahmen-DeVore-Nichols,2020).

Given $(\Omega, \mathcal{F}, \mathbb{P})$ some probability space, we assume

$$\Delta(u_n(\xi), \xi) := \|u(\xi) - u_n(\xi)\|_V^2 = \mathbb{E}(Z_n(\xi)), \tag{5}$$

where $Z_n(\xi)$ is some parameter-dependent real valued random variable.

Probabilistic greedy algorithm

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Algorithm 2: Probabilistic greedy algorithm

Start from $V_0 = \{0\}$ and proceed, for $n \geq 1$, as follows.

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$$\xi_n \in \mathcal{S}(Z_{n-1}(\xi), \tilde{\Xi})$$

2) Compute $u(\xi_n)$ and update $V_n = \text{span}\{u(\xi_1), \dots, u(\xi_n)\}$.

How to choose the "(random) set of candidate parameter values" $\mathcal{S}(Z_{n-1}(\xi), \tilde{\Xi})$?

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Probabilistic construction of reduced space.

- Greedy algorithm with random training sets for : high-dimensional parameter-dependent problems (Cohen,2020), for EIM (Cai,2022)
- MC-greedy algorithm for control variate method within RB paradigm (Boyaval-Lelièvre,2010) (Blel-Ehrlacher-Lelièvre,2021)

Crude Monte-Carlo estimate based approach.

Seek ξ_n as the maximum of the empirical mean i.e.

$$\mathcal{S}(Z_{n-1}(\xi),\tilde{\Xi}) := \arg\max_{\xi\in\tilde{\Xi}} \overline{Z_{n-1}(\xi)}_K$$

where $\overline{Z_{n-1}(\xi)}_K = \frac{1}{K}\sum_{i=1}^{K}(Z_{n-1}(\xi))_i$ with K i.i.d. copies of $Z_{n-1}(\xi)$.

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- ✓ Practically simple.
- ✗ Slow convergence of the estimate with respect to the number of samples.
- ✗ High computational costs especially if $Z_{n-1}(\xi)$ is expensive to evaluate.
- ✗ No guarantee that ξ_n (random) is a (quasi-)optimum, almost surely or at least with high probability.

Bandit algorithms based approach. Bandit algorithms are good candidates.

$$\mathcal{S}(Z_{n-1}(\xi), \tilde{\Xi}) := \mathrm{PAC}_{\lambda_n,\varepsilon}(Z_{n-1}, \tilde{\Xi})$$

with threshold ε in $(0,1)$ and probability of failure λ_n in $(0,1)$.

(Lattimore-Szepesvári,2022)

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(Lattimore-Szepesvári,2022)

✓ Designed to return a probably approximately correct (PAC) maximum ξ_n in relative precision

$$\mathbb{P}\left(\mathbb{E}(Z_{n-1}(\xi_n^\star)) - \mathbb{E}(Z_{n-1}(\xi_n)) \leq \varepsilon \mathbb{E}(Z_{n-1}(\xi_n^\star))\right) \geq 1 - \lambda_n, \tag{6}$$

for any prescribed threshold ε in $(0,1)$, probability of failure λ_n in $(0,1)$ and

$$\xi_n^\star \in \arg\max_{\xi \in \tilde{\Xi}} \mathbb{E}[Z_{n-1}(\xi)].$$

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(Billaud-Macherey-Nouy-Prieur,2022)

✓ Adaptive number of samples.

✗ Requires strong assumptions on the distribution of $Z_{n-1}(\xi)$ leading to practical limitations.

Appendix 1

Theorem (Billaud-Macherey-Nouy-Prieur,2023)

Take $(\lambda_n)_{n\geq 1} \in (0,1)$ such that $\sum_{n\geq 1} \lambda_n = \lambda < 1$, $\varepsilon \in (0,1)$ and $\tilde{\Xi} \subset \Xi$ a discrete training set. Moreover, suppose that for $n \geq 1$, the approximation u_n of u in V_n is quasi-optimal

$$\|u(\xi) - u_n(\xi)\|_V \leq C\|u(\xi) - P_{V_n} u(\xi)\|_V, \quad \xi \in \tilde{\Xi}, \tag{7}$$

for some constant C independent from V_n and ξ. Then, Algorithm 2 with PAC based approach is a weak-greedy algorithm of parameter $\frac{\sqrt{1-\varepsilon}}{C}$, with probability at least $1-\lambda$ i.e.

$$\mathbb{P}\left(\|u(\xi_n) - P_{V_{n-1}} u(\xi_n)\|_V \geq \frac{\sqrt{1-\varepsilon}}{C} \max_{\xi \in \tilde{\Xi}} \|u(\xi) - P_{V_{n-1}} u(\xi)\|_V, \forall n \geq 1\right) \geq 1-\lambda. \tag{8}$$

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Let $D \subset \mathbb{R}^d$ be an open bounded domain with boundary ∂D. We want to approximate

$$u(\xi) : D \to \mathbb{R}$$

from its pointwise evaluations in D.

Offline stage. Use the probabilistic greedy algorithm to construct V_n with

$$\Delta(u_n(\xi), \xi) = \|u_n(\xi) - u(\xi)\|^2_{L^2(D)} = \mathbb{E}(Z_n(\xi))$$

with $Z_n(\xi) = |D||u(Y, \xi) - u_n(Y, \xi)|^2$ where $Y \sim \mathcal{U}(D)$.

Online stage. The approximation $u_n(\xi)$ is an interpolant of $u(\xi)$ in V_n

$$u_n(x_i, \xi) = u(x_i, \xi), \;\; x_i \in \Gamma,$$

with $\Gamma = \{x_1, \dots, x_n\}$ an unisolvant grid of interpolation points in D for V_n (e.g. the magic points).

- D : deterministic RBM with

$$\xi_n \in \arg\max_{\xi \in \tilde{\Xi}} \|u(\xi) - u_n(\xi)\|^2_{L^2(D)}.$$

The L^2-norm is estimated by trapezium rule with grid $\tilde{D}$.

- MC : probabilistic RBM with MC estimate

$$\xi_n \in \arg\max_{\xi \in \tilde{\Xi}} \overline{Z_{n-1}(\xi)}_K.$$

We set $K \in \{1, 50\}$.

- PAC : probabilistic RBM with PAC selection

$$\xi_n \in \arg\max_{\xi \in \tilde{\Xi}} \mathrm{PAC}_{\lambda,\varepsilon}(Z_{n-1}(\xi), \tilde{\Xi}).$$

  with asymptotic (TCL) or non asymptotic (Bounded) concentrations inequalities.

  The probability of failure is $\lambda = 0.1$ and stopping criterion $\varepsilon = 0.9$.

- R : RBM with ξ_n chosen at random in $\tilde{\Xi}$ without replacement.

Test case 1.

$$u(x,\xi) = 10x\sin(2\pi x\xi),\ \ (x,\xi) \in [0,1]\times[2,4]$$

Reduced space dimension $n = 20$. Training sets : $\#\tilde{\Xi} = 300$, $\#\tilde{D} = 10000$.

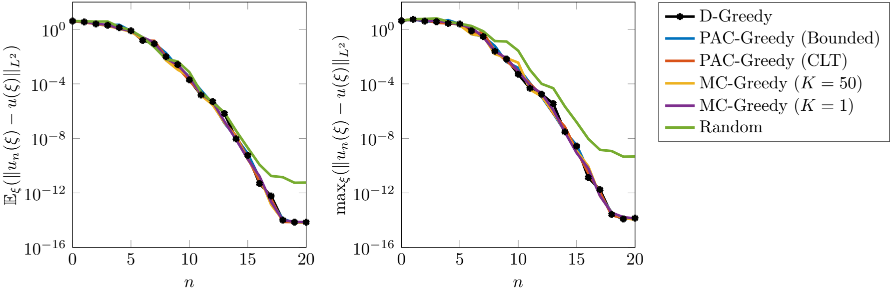

Figure Evolution with n of the estimated maximum of approximation error for 100 instances of ξ, for one realisation of the probabilistic greedy algorithms compared to the deterministic one.

Numerical results

Test case 2.

$$u(x,\xi) = \sqrt{x+0.1}\,\mathbf{1}_{[0,\xi]}(x) + \left(\frac{x-\xi}{2\sqrt{\xi+0.1}} + \sqrt{\xi+0.1}\right)\mathbf{1}_{[\xi,1]}(x), \quad (x,\xi)\in[0,1]^2$$

Reduced space dimension $n = 30$. Training sets : $\#\tilde{\Xi} = 300$, $\#\tilde{D} = 1000$.

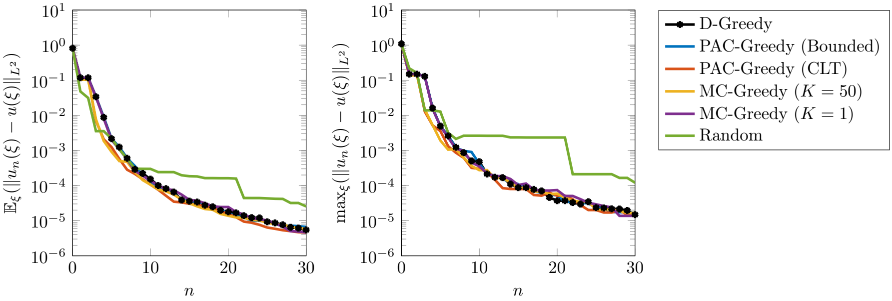

Figure Evolution with n of the estimated maximum of approximation error for 100 instances of ξ, for one realisation of the probabilistic greedy algorithms compared to the deterministic one.

$\Rightarrow$ Best trade-off between efficiency and accuracy : MC-Greedy ($K = 1$).

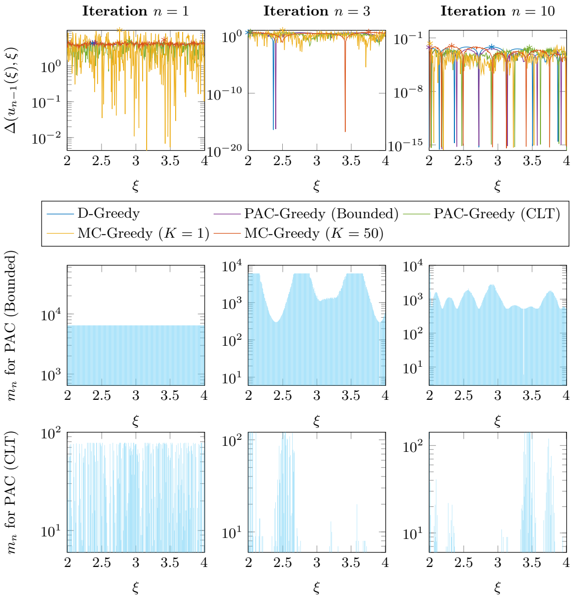

Figure (TC1) Evolution of the error during greedy procedures based on PAC bandit algorithms (top), together with required samples $m_n(\xi)$ for selecting $\xi_n \in \tilde{\Xi}$.

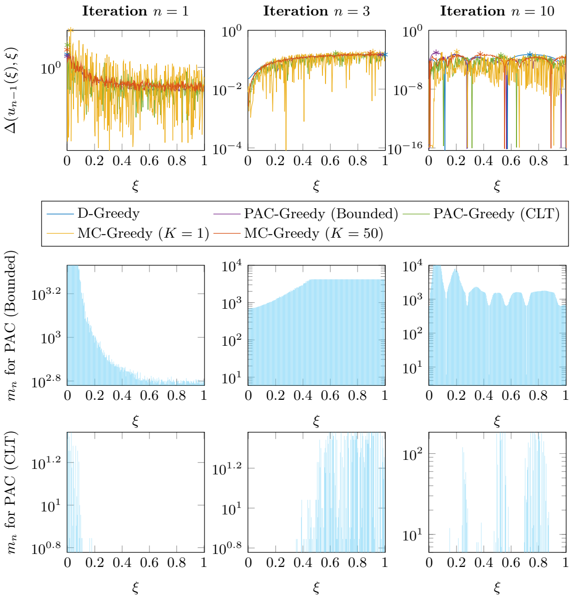

Figure (TC2) Evolution of the error during greedy procedures based on PAC bandit algorithms (top), together with required samples $m_n(\xi)$ for selecting $\xi_n \in \tilde{\Xi}$.

Method	(TC1) for $n = 20$	(TC2) for $n = 30$
D-Greedy	6×10^7	9×10^6
MC-Greedy $K = 1$	6×10^3	9×10^3
MC-Greedy $K = 50$	3×10^5	4.5×10^5
PAC-Greedy (Bounded)	1.284326×10^7	5.764507×10^7
PAC-Greedy (CLT)	7.507800×10^4	2.333380×10^5

Table Cumulative number of samples required by each algorithm, for (TC1) and (TC2), to construct reduced basis of dimension n.

Let $D \subset \mathbb{R}^d$ be an open bounded domain with boundary ∂D. We seek, for all $\xi \in \Xi$, $u(\xi) : D \to \mathbb{R}$ solution of

$$\begin{aligned} -\mathcal{A}(\xi)u(\xi) &= g(\xi), \quad \text{in } D, \\ u(\xi) &= f(\xi), \quad \text{on } \partial D, \end{aligned} \tag{9}$$

with given functions $g : \bar{D} \times \Xi \to \mathbb{R}$ and $f : \partial D \times \Xi \to \mathbb{R}$.

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The parameter-dependent elliptic partial differential operator $\mathcal{A}(\xi)$ is defined as

$$\mathcal{A}(\xi) = \frac{1}{2} \sum_{i,j=1}^{d} (\sigma(\xi)\sigma(\xi)^T)_{ij} \partial^2_{x_i x_j} + \sum_{i=1}^{d} b_i(\xi) \partial_{x_i},$$

with parameter-dependent drift $b : \mathbb{R}^d \times \Xi \to \mathbb{R}^d$ and diffusion $\sigma : \mathbb{R}^d \to \mathbb{R}^{d \times d}$.

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A classical framework.

It is usually considered :

- an approximated problem (9) for a given mesh of D (e.g. finite element...),
- $u_n(\xi)$ obtained through suitable projection (e.g. galerkin, least-square...) using the equation residual,
- $\Delta(u_n(\xi), \xi)$ related to some norm of the equation residual.

What if we can access to pointwise values (noisy) of $u(x, \xi)$ for any $(x, \xi) \in D \times \Xi$?

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Probabilistic and sample based framework.

We could consider :

- global approximation over D of the solution of (9) obtained from pointwise values (noisy) (e.g. interpolation, least-square...)

  $\rightsquigarrow$ snapshots, approximation $u_n(\xi)$ avoiding the use of equation residual,
- use a probabilistic greedy algorithm with $\Delta(u_n(\xi), \xi)$ related to some norm of the current error.

The operator $\mathcal{A}(\xi)$ is the infinitesimal generator related to the diffusion process $X^{x,\xi} = (X_t^{x,\xi})_{t\geq 0}$ satisfying the following SDE

$$dX_t^{x,\xi} = b(X_t^{x,\xi}, \xi)dt + \sigma(X_t^{x,\xi}, \xi)\ dW_t, \quad X_0^{x,\xi} = x \in \overline{D}, \tag{10}$$

$W = (W_t)_{t\geq 0}$ is a d-dimensional brownian motion on $(\Omega, \mathcal{F}, \mathbb{P})$ endowed with its natural filtration $(\mathcal{F}_t)_{t\geq 0}$.

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Feynman-Kac (FK) formula (Friedman (§6,Theorem 2.4),2010)

Under suitable assumptions on $f(\xi), g(\xi)$ and $b(\xi), \sigma(\xi)$ Appendix 2 there exists a unique solution $u(\xi)$ of (9) in $\mathcal{C}\left(\overline{D}\right) \cap \mathcal{C}^2\left(D\right)$, which satisfies for all $x \in \overline{D}$

$$u(x,\xi) = \mathbb{E}(F(x,X^{x,\xi},\xi)) := \mathbb{E}\left(f(X_{\tau^{x,\xi}}^{x,\xi},\xi) + \int_0^{\tau^{x,\xi}} g(X_t^{x,\xi},\xi)dt\right), \tag{11}$$

where $X^{x,\xi}$ is diffusion process solution of (10) stopped at $t = \tau^{x,\xi}$.

The operator $\mathcal{A}(\xi)$ is the infinitesimal generator related to the diffusion process $X^{x,\xi} = (X_t^{x,\xi})_{t\geq 0}$ satisfying the following SDE

$$dX_t^{x,\xi} = b(X_t^{x,\xi}, \xi)dt + \sigma(X_t^{x,\xi}, \xi)\ dW_t, \quad X_0^{x,\xi} = x \in \overline{D}, \tag{10}$$

$W = (W_t)_{t\geq 0}$ is a d-dimensional brownian motion on $(\Omega, \mathcal{F}, \mathbb{P})$ endowed with its natural filtration $(\mathcal{F}_t)_{t\geq 0}$.

Feynman-Kac (FK) formula (Friedman (§6,Theorem 2.4),2010)

Under suitable assumptions on $f(\xi), g(\xi)$ and $b(\xi), \sigma(\xi)$ Appendix 2 there exists a unique solution $u(\xi)$ of (9) in $\mathcal{C}\left(\overline{D}\right) \cap \mathcal{C}^2\left(D\right)$, which satisfies for all $x \in \overline{D}$

$$u(x,\xi) = \mathbb{E}(F(x, X^{x,\xi}, \xi)) := \mathbb{E}\left(f(X_{\tau^{x,\xi}}^{x,\xi}, \xi) + \int_0^{\tau^{x,\xi}} g(X_t^{x,\xi}, \xi)dt \right), \tag{11}$$

where $X^{x,\xi}$ is diffusion process solution of (10) stopped at $t = \tau^{x,\xi}$.

In practice. Appendix 3

Monte-Carlo estimates of $u(x,\xi)$ can be computed from i.i.d. realizations of an approximation of $X^{x,\xi}$ (e.g. computed with Euler-Maruyama scheme).

We consider

$$\Delta(u_n(\xi), \xi) = \|u(\xi) - u_n(\xi)\|^2_{L^2(D)}.$$

Since (9) is linear

$$\begin{aligned} -\mathcal{A}(\xi)(u(\xi) - u_n(\xi)) &= g_n(\xi) \quad \text{on} \quad D, \\ u(\xi) - u_n(\xi) &= f_n(\xi) \quad \text{on} \quad \partial D, \end{aligned} \tag{12}$$

where $f_n(\xi) := f(\xi) - u_n(\xi)$ and $g_n(\xi) = g(\xi) + \mathcal{A}(\xi)u_n(\xi)$. For all $x \in \bar{D}$, by FK theorem,

$$u(x,\xi) - u_n(x,\xi) = \mathbb{E}\left(F_n(x, X^{x,\xi}, \xi)\right) := \mathbb{E}\left(f_n(X^{x,\xi}_{\tau^{x,\xi}}, \xi) + \int_0^{\tau^{x,\xi}} g_n(X^{x,\xi}_t, \xi) dt\right). \tag{13}$$

Probabilistic error estimate

We consider

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Theorem (Billaud-Macherey-Nouy-Prieur,2023)

Taking $Y \sim U(D)$, we have for all ξ in Ξ

$$\|u(\xi) - u_n(\xi)\|^2_{L^2(D)} = |D|\mathbb{E}\left(Z_n(\xi)\right), \text{ with } \quad Z_n(\xi) := F_n(Y, X^{Y,\xi},\xi)F_n(Y,\tilde{X}^{Y,\xi},\xi), \tag{14}$$

with $X^{Y,\xi}$, $\tilde{X}^{Y,\xi}$ two diffusion processes solutions of (10) starting from Y.

Numerical results

Problem. We seek $u(\xi)$ solution on $D =]0,1[$ of the following one dimensional PDE

$$-\mathcal{A}(\xi) = -\xi u''(\xi) + 10u'(\xi) = g(\xi) \text{ in } D, \qquad u(\xi) = f(\xi) \text{ at } x = 0, 1, \qquad (15)$$

The functions $g(\xi)$ and $f(\xi)$ are set such that the exact solution is known

$$u(x,\xi) = \frac{\exp(x/\xi) - 1}{\exp(1/\xi) - 1}, \quad \xi \in [0.005, 1].$$

Snapshots are computed using the exact solution.

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Approximation setting.

Interpolation v.s. Least-Square (LS) v.s. Minimal Residual (MinRes)

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Interpolation v.s. Least-Square (LS) v.s. Minimal Residual (MinRes)

Confronted greedy approaches.

- Residual : deterministic alg. based on the L^2-norm of the eq. residual

$$\|\mathcal{A}(\xi) + g(\xi)\|_{L^2(D)}$$

- FK-MC : probabilistic alg. with MC estimate based on FK error interpretation

$$\|u(\xi) - u_n(\xi)\|^2_{L^2(D)} = |D|\mathbb{E}\left(Z_n(\xi)\right)$$

  with $Z_n(\xi) := F_n(Y, X^{Y,\xi}, \xi)F_n(Y, \tilde{X}^{Y,\xi}, \xi)$
- Random : snapshots chosen at random in $\tilde{\Xi}$ without replacement

Numerical results

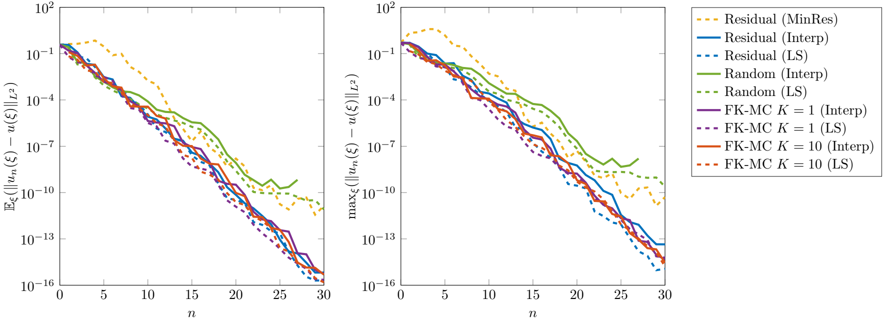

Figure Evolution with respect to n, of the estimated maximum of the approximation error in L^2-norm, computed for 100 instances of ξ, for one realisation of the probabilistic greedy algorithms compared to the deterministic one.

Probabilistic RBM in sample setting.

- Greedy algorithm with probabilistic error (even with coarse MC estimate) demonstrates to provide good reduced spaces.
- Sample based projections improves the global approximation quality by avoiding the use of residual.

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Perspectives.

✓ Interpolation with FK pointwise evaluation (Billaud-Friess, Macherey, Nouy, Prieur,2020), (Gobel, Maire,2006) to avoid limitations of residual based projections Appendix 4

✗ ... but how to provide a a projection with controlled error and at low cost ?

✗ Extension to more complex and higher dimension problems.

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Thanks for attention !

M. Billaud-Friess, A. Macherey, A. Nouy, C. Prieur, A probabilistic reduced basis method for parameter-dependent problems, ArXiv :2304.08784 (to appear in ACOM).

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Here $\{Z(\xi) : \xi \in \tilde{\Xi}\}$ is a finite collection of random variables with $\mathbb{E}[Z(\xi)] \neq 0$.
We denote

$$\overline{Z(\xi)}_m = \frac{1}{m} \sum_{k=1}^{m} Z(\xi)_k \quad \text{and} \quad \overline{V(\xi)}_m = \frac{1}{m} \sum_{k=1}^{m} \left(Z(\xi)_k - \overline{Z(\xi)}_m \right)^2, \tag{16}$$

where $Z(\xi)_1, \ldots, Z(\xi)_m$ are m independent copies of $Z(\xi)$.
The random variable $Z(\xi)$ is assumed to satisfy the following (possibly asymptotic) concentration inequality

$$\mathbb{P}\left(|\overline{Z(\xi)}_m - \mathbb{E}[Z(\xi)]| \leq c(m, x, \xi) \right) \geq 1 - x, \tag{17}$$

for each $\xi \in \tilde{\Xi}$, $0 \leq x \leq 1$ and $m \geq 1$.
If for any $\xi \in \tilde{\Xi}$, there exists $a(\xi), b(\xi) \in \mathbb{R}$ such that almost surely we have $a(\xi) \leq Z(\xi) \leq b(\xi)$, then (17) holds with

$$c(m, x, \xi) = \sqrt{\frac{2\overline{V(\xi)}_m \log(3/x)}{m}} + \frac{3\,(b(\xi) - a(\xi)) \log(3/x)}{m}.$$

Now, let us define a sequence $(d_m)_{m\geq 1} \subset (0,1)^{\mathbb{N}}$, independent from ξ, and such that $\sum_{m\geq 1} d_m < \infty$.
Then we introduce $c_{\xi,m} = c(m, d_m, \xi)$, and $\beta^{\pm}_{\xi,m(\xi)} = \overline{Z(\xi)}_{m(\xi)} \pm c_{\xi,m(\xi)}$.
Letting $s(\xi) := \text{sign}(\overline{Z(\xi)}_{m(\xi)})$ and $\varepsilon_{\xi,m(\xi)} = \begin{cases} \frac{c_{\xi,m(\xi)}}{|\overline{Z(\xi)}_{m(\xi)}|} & \text{if } \overline{Z(\xi)}_{m(\xi)} \neq 0, \\ +\infty & \text{otherwise.} \end{cases}$, we define the following estimate for $\mathbb{E}[Z(\xi)]$ given by

$$\hat{\mathbb{E}}_{m(\xi)}[Z(\xi)] = \begin{cases} \overline{Z(\xi)}_{m(\xi)} - \varepsilon_{\xi,m(\xi)} \; s(\xi) c_{\xi,m(\xi)} & \text{if } \varepsilon_{\xi,m(\xi)} < 1, \\ \overline{Z(\xi)}_{m(\xi)} & \text{otherwise.} \end{cases} \tag{18}$$

Appendix 1 : Adaptive PAC algorithm

Adaptive bandit algorithm (Billaud-Macherey-Nouy-Prieur,2022)

Let $\varepsilon, \lambda \in (0,1)$ and $K \in \mathbb{N}$. Set $\ell = 0$, $\Xi_0 = \tilde{\Xi}$, $m(\xi) = K$ and $\varepsilon_{\xi,m(\xi)} = +\infty$ for all $\xi \in \Xi$.
while $\#\Xi_\ell > 1$ **and** $\max\limits_{\xi \in \Xi_\ell} \varepsilon_{\xi,m(\xi)} > \frac{\varepsilon}{2+\varepsilon}$ **do**
  for all $\xi \in \Xi_\ell$ **do**
    Sample $Z(\xi)$, increment $m(\xi)$ and update $\varepsilon_{\xi,m(\xi)}$.
    Compute the estimate $\hat{\mathbb{E}}_{m(\xi)}[Z(\xi)]$ using (18).
  end for
  Increment ℓ and put in Ξ_ℓ every $\xi \in \tilde{\Xi}$ such that

$$\beta^+_{\xi,m(\xi)} \geq \max_{\nu \in \tilde{\Xi}} \beta^-_{\nu,m(\nu)}. \tag{19}$$

end while
Select $\hat{\xi}$ such that

$$\hat{\xi} \in \arg\max_{\xi \in \Xi_\ell} \hat{\mathbb{E}}_{m(\xi)}\left[Z(\xi)\right].$$

At each step ℓ, the number of samples $m(\xi)$ of the random variables $Z(\xi)$ is increased in the subset $\Xi_\ell \subset \tilde{\Xi}$, obtained using confidence intervals $[\beta^-_{m(\xi)}(\xi), \beta^+_{m(\xi)}(\xi)]$ of $\mathbb{E}(Z(\xi))$ according to (19). The idea is to find regions of $\tilde{\Xi}$ where one has a high chance to find a maximum.

Dependence to ξ is omitted to alleviate notations.

- There exists a constant $0 < M < +\infty$ such that for all $x, y \in \bar{D}$ we have

$$\|b(x) - b(y)\| + \|\sigma(x) - \sigma(y)\| \leq M\|x - y\|, \tag{20}$$

- Denoting $a = \sigma\sigma^T$, there exists $c > 0$ such that

$$y^T a(x) y \geq c\|y\|^2, \quad y \in \mathbb{R}^d,\ x \in \overline{D}.$$

- As problem (9) is defined on a bounded domain, we define the first exit time of D for the process X^x as

$$\tau^x = \inf\{s > 0 \ : \ X_s^x \notin D\}. \tag{21}$$

- The domain D is an open connected bounded domain of $\mathbb{R}^d$, regular in the sense that it satisfies the following conditions
  i)
  $$\mathbb{P}(\tau^x = 0) = 1, \quad x \in \partial D,$$
  ii) each point of ∂D satisfies the exterior cone condition which means that, for all $x \in \partial D$, there exists a finite right circular cone K, with vertex x, such that $\overline{K} \cap \overline{D} = \{x\}$.
- We assume that f is continuous on ∂D, g is Hölder-continuous on $\overline{D}$.

Appendix 3 : Pointwise estimate $u_{\Delta t,M}(x,\xi)$

We consider the time mesh $0 = t_0 < \cdots < t_n < \dots$, with $t_n = n\Delta t,\ n \in \mathbb{N}$.

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Maruyama scheme for computing $X^{x,\Delta t}$.

The diffusion process X^x is approximated by a piecewise constant process $X^{x,\Delta t}$, where $X_t^{x,\Delta t} = X_n^{x,\Delta t}$ for $t \in [t_n, t_{n+1}[$ and

$$\begin{aligned} X_{n+1}^{x,\Delta t} &= X_n^{x,\Delta t} + \Delta t\ b(X_n^{x,\Delta t}) + \sigma(X_n^{x,\Delta t})\ \Delta W_n, \\ X_0^{x,\Delta t} &= x, \end{aligned} \tag{22}$$

where $\Delta W_n = W_{n+1} - W_n$ is an increment of the standard Brownian motion.

Approximated stopping time $\tau^{x,\Delta t}$.

We consider

$$\tau^{x,\Delta t} = \min\left\{ t_n > 0 \ : \ X_{t_n}^{x,\Delta t} \notin D \right\}. \tag{23}$$

Monte Carlo estimate $u_{\Delta t,M}(x)$ of $u(x)$.

For $x \in \bar{D}$ and $\{X^{x,\Delta t}(\omega_m)\}_{m=1}^{M}$ independent samples of $X^{x,\Delta t}$, we consider

$$u_{\Delta t,M}(x) = \frac{1}{M} \sum_{m=1}^{M} \left[f(X_{\tau^{x,\Delta t}}^{x,\Delta t}(\omega_m)) + \int_0^{\tau^{x,\Delta t}} g(X_t^{x,\Delta t}(\omega_m)) dt \right]. \tag{24}$$

We seek a global approximation of u from the pointwise estimates $u_{\Delta t,M}(x)$, $x \in \bar{D}$.

Linear approximation. Consider the approximation space $V_m \subset \mathcal{C}^2(\overline{D})$ of dim. m and

$$\mathcal{L}_m : \mathcal{C}^2(\overline{D}) \to V_m$$

the approximation operator associated with a grid $\Gamma = \{x_i\}_{i=1}^p \subset \bar{D}$ with $p \geq m$.

Exemples : Interpolation ($p = m$), least-square approximation

Naive approach. Choose an approximation for u as

$$\tilde{u} = \mathcal{L}_m(u_{\Delta t,M}).$$

$\rightsquigarrow$ It may suffer from the slow convergence of MC estimates w.r.t. M.

(Gobet, Maire,2006)

Construct a sequence of approximations $\{\tilde{u}^k\}_{k\geq 1}$ of u in V_m as

$$\tilde{u}^k = \tilde{u}^{k-1} + \tilde{e}^k, \qquad k \geq 1,$$

where $\tilde{e}^k \approx e^k = u - \tilde{u}^{k-1}$, solution of

$$\begin{aligned} -\mathcal{A}e^k(x) &= g(x) + \mathcal{A}\tilde{u}^{k-1}(x), && x \in D, \\ e^k(x) &= f(x) - u^{k-1}(x), && x \in \partial D. \end{aligned}$$

Since e^k admits the Feyman-Kac representation

$$e^k(x) = \mathbb{E}\left((f - \tilde{u}^{k-1})(X^x_{\tau^x}) + \int_0^{\tau^x} (g + \mathcal{A}\tilde{u}^{k-1})(X^x_t) dt \right),$$

we can compute

$$\tilde{e}^k = \mathcal{L}_m(e^k_{\Delta t, M}).$$

Remarks.

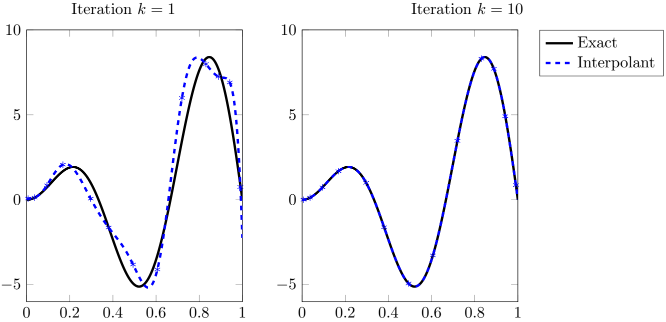
- ✓ For interpolation, the $u - \tilde{u}^k$ converges geometrically to zero up to a threshold term depending on Δt and interpolation error (Gobet, Maire,2006)
- ✓ For high-dimensional problems with sparse interpolation (B.-F., Macherey, Nouy, Prieur,2020)

We seek $u(\xi)$ solution on $D =]0,1[$ of the following one dimensional PDE

$$-\mathcal{A}u = -3\pi u'' - bu' = g \text{ in } D, \qquad u = f \text{ at } x = 0, 1, \tag{25}$$

The functions $g(\xi)$ and $f(\xi)$ are set s.t. $u(x) = 10x sin(3\pi x)$. The associated SDE is

$$dX_t^x = bdt + \sqrt{6\pi} dW_t, \qquad X_0^x = x.$$



Interpolation of using B-Splines ($\mathbb{P}_4$), $\dim V_m = 13$ for a grid Γ of Magic Points.
Sequential control variate algorithm with $M = 100$, $k_{max} = 10$ and $\Delta t = 10^{-4}$.