Introduction to greedy algorithms for high-dimensional problems

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Motivation

High-dimensional problems are ubiquitous: quantum mechanics, kinetic models, molecular dynamics, uncertainty quantification, finance, multiscale models etc.

How to compute $u(x_1, \cdots, x_d)$ with d potentially large?

The bottom line of deterministic approaches is to represent solutions as linear combinations of tensor products of small-dimensional functions (parallelepipedic domains):

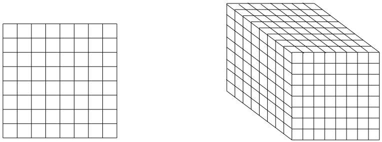
$$\begin{aligned} u(x_1, \cdots, x_d) &= \sum_{k \geq 1} r_k^1(x_1) r_k^2(x_2) \cdots r_k^d(x_d) \\ &= \sum_{k \geq 1} \left(r_k^1 \otimes r_k^2 \otimes \cdots \otimes r_k^d \right)(x_1, x_2, \cdots, x_d). \end{aligned}$$

Curse of dimensionality

Classical approach: Galerkin method using standard finite element discretization with N degrees of freedom per variate.

$$u(x_1, \cdots, x_d) \approx \sum_{(i_1,\cdots,i_d)\in\{1,\cdots,N\}^d} \lambda_{i_1,\cdots,i_d} \left(\phi^1_{i_1} \otimes \cdots \otimes \phi^d_{i_d}\right)(x_1, \cdots, x_d),$$

where the basis functions $\left(\phi^j_i\right)_{1\leq i\leq N,\, 1\leq j\leq d}$ are chosen a priori and the real numbers $(\lambda_{i_1,\cdots,i_d})_{1\leq i_1,\cdots,i_d\leq N}$ are to be computed.



$$DIM = N^d$$

This is the so-called curse of dimensionality ([Bellman, 1957])

Greedy algorithms

Progressive Generalized Decomposition: Here, we consider an approach proposed by:

- Ladevèze *et al.* to do time-space variable separation;
- Chinesta *et al.* to solve high-dimensional Fokker-Planck equations in the context of kinetic models for polymers;
- Nouy *et al* in the context of uncertainty quantification.

They are related to the so-called greedy algorithms introduced in nonlinear approximation theory: ([Temlyakov, 2008], Cohen, DeVore, Dahmen, Maday...)

The idea is to look iteratively for the best tensor product:

$$u(x_1, \dots, x_d) \approx \sum_{k=1}^{n} \left(r_k^1 \otimes r_k^2 \otimes \cdots \otimes r_k^d\right)(x_1, x_2, \dots, x_d).$$

$$\boxed{DIM = n \times Nd}$$

Outline

Outline

Minimization problem

Let us consider for simplicity the case of only two variables: $u(x, y) \in V$, with V a Hilbert space of functions depending on the two variables x and y. The algorithm and all the results below generalize to the case of tensor products of more than two functions.

Let us introduce a functional $\mathcal{E} : V \to \mathbb{R}$ with a unique global minimizer:

$$\boxed{u = \underset{v \in V}{\text{argmin}}\, \mathcal{E}(v),}$$

and the set of tensor product functions

$$\Sigma := \{r \otimes s,\ r \in V_x,\ s \in V_y\}, \tag{1}$$

where V_x (respectively V_y) is a Hilbert space of functions depending **only** on the variable x (respectively on the variable y) such that

$$\text{Span}\Sigma \subset V.$$

We wish to approximate the function $u(x, y)$ as

$$u(x, y) = \sum_{k \geq 1} r_k(x) s_k(y), \quad \text{where for all } k \in \mathbb{N}^*,\ r_k \in V_x,\ s_k \in V_y.$$

Definition of the Pure Greedy algorithm for unconstrained minimization problems

The so-called Pure Greedy algorithm reads:

1. set $u_0 = 0$ and $n = 1$;
2. find $(r_n, s_n) \in V_x \times V_y$ such that

$$(r_n, s_n) \in \underset{r \in V_x,\, s \in V_y}{\operatorname{argmin}} \mathcal{E}\left(u_{n-1} + r \otimes s\right).$$

3. set $u_n = u_{n-1} + r_n \otimes s_n$ and $n = n + 1$. Return to step 2.

At the n^{th} iteration of the algorithm, we have

$$u_n = \sum_{k=1}^{n} r_k \otimes s_k.$$

Question: Are the iterations of the algorithm well-defined and does $(u_n)_{n \in \mathbb{N}^*}$ converge towards u?

Main assumptions

[Le Bris, Lelièvre, Maday, 2009], [Cancès, VE, Lelièvre, 2011], [Nouy, Falco, 2011]

Assumptions:

(Σ1) Span$\Sigma \subset V$ is dense;

(Σ2) Σ is weakly closed in V;

(E1) $\mathcal{E}$ is differentiable on V and its gradient is Lipschitz on bounded sets, i.e.

$$\forall K \text{ bdd } \subset V, \exists L_K > 0, \forall v, w \in K, \; \|\mathcal{E}'(v) - \mathcal{E}'(w)\|_V \leq L_K \|v - w\|_V.$$

(E2) there exists $\alpha > 0$ and $s > 1$ such that

$$\forall v, w \in V, \; \langle \nabla\mathcal{E}(v) - \nabla\mathcal{E}(w), v - w \rangle_V \geq \frac{\alpha}{2} \|v - w\|_V^s.$$

The quadratic case and prototypical example

In particular, when for all $v \in V$,

$$\mathcal{E}(v) = \frac{1}{2}a(v,v) - l(v),$$

with $a : V \times V \to \mathbb{R}$ is a **symmetric continuous coercive** and $l : V \to \mathbb{R}$ is a continuous linear form, $\mathcal{E}$ satisfies (E1) and (E2).

Example: $V = H_0^1(\Omega_x \times \Omega_y)$, with Ω_x, Ω_y open regular bounded subsets of $\mathbb{R}$, $f \in L^2(\Omega_x \times \Omega_y)$.

$$\mathcal{E}(v) := \frac{1}{2}\int_{\Omega_x \times \Omega_y} |\nabla_{x,y} v|^2 - \int_{\Omega_x \times \Omega_y} fv.$$

The unique global minimizer $u = \mathrm{argmin}_{v \in V}\, \mathcal{E}(v)$ is the unique solution $u \in H_0^1(\Omega_x \times \Omega_y)$ of

$$-\Delta_{x,y} u = f \text{ in } \mathcal{D}'(\Omega_x \times \Omega_y).$$

With $V_x := H_0^1(\Omega_x)$, $V_y := H_0^1(\Omega_y)$, Σ defined by (1) satisfies (Σ1) and (Σ2).

Convergence results

$$(r_n, s_n) \in \underset{(r,s)\in V_x \times V_y}{\text{argmin}} \ \mathcal{E}\left(u_{n-1} + r \otimes s\right) \tag{2}$$

Theorem

Under assumptions (Σ1), (Σ2), (E1) et (E2), the iterations of the Pure Greedy algorithm are well-defined (i.e. there exists at least one minimizer (r_n, s_n) to (2) for all $n \in \mathbb{N}^*$ and $r_n \otimes s_n$ is non-zero if and only if $u_{n-1} \neq u$). Moreover, the sequence $(u_n)_{n\in\mathbb{N}^*}$ strongly converges in V towards u.

Theorem

In the case when the Hilbert space V is finite-dimensional, the convergence is exponentially fast: $\exists C > 0, \sigma \in (0,1)$,

$$\|u - u_n\|_V \leq C\sigma^n.$$

Practical implementation

The Euler equations associated to (2) in the quadratic case read: for all $(\delta r, \delta s) \in V_x \times V_y$,

$$a(u_n, r_n \otimes \delta s + \delta r \otimes s_n) = l(r_n \otimes \delta s + \delta r \otimes s_n).$$

Return to the Laplacian example: At the n^{th} iteration of the greedy algorithm, $(r_n, s_n) \in V_x \times V_y$ are solutions of

$$\left\{ \begin{array}{l} \left(\int_{\Omega_y} |s_n|^2\right)(-\Delta_x r_n) + \left(\int_{\Omega_y} |\nabla_y s_n|^2\right) r_n = \int_{\Omega_y} f_{n-1}(\cdot, y), s_n(y)\, dy, \\ \left(\int_{\Omega_x} |r_n|^2\right)(-\Delta_y s_n) + \left(\int_{\Omega_x} |\nabla_x r_n|^2\right) s_n = \int_{\Omega_x} f_{n-1}(x, \cdot), r_n(x)\, dx. \end{array} \right.$$

where $f_{n-1} := f + \Delta_{x,y} u_{n-1}$.

Coupled nonlinear problem: usually solved via a fixed-point procedure.

Definition of the Pure Greedy algorithm for general dictionaries

[Nouy, Falco, 2011]

$\Sigma \subset V$ satisfying $(\Sigma 1)$, $(\Sigma 2)$ and

$(\Sigma 3)$ Σ is a non-empty cone, i.e. $0 \in \Sigma$ and for all $(t, z) \in \mathbb{R} \times \Sigma$, $tz \in \Sigma$.

Any tensor format satisfying these assumptions (Hackbusch, Khoromskij, Kolda Bader, Beylkin, Mohlenkamp...) can be used instead of rank-1 tensor products.

The so-called Pure Greedy algorithm reads:

1. set $u_0 = 0$ and $n = 1$;
2. find $z_n \in \Sigma$ such that
$$z_n \in \operatorname*{argmin}_{z \in \Sigma} \mathcal{E}\left(u_{n-1} + z\right).$$
3. set $u_n = u_{n-1} + z_n$ and $n = n + 1$. Return to step 2.

The two previous theorems also hold in this case!

Orthogonal Greedy algorithm

[Le Bris, Lelièvre, Maday, 2009], [Nouy, Falco, 2011]

The so-called Orthogonal Greedy algorithm reads:

1. set $u_0 = 0$ and $n = 1$;
2. find $z_n \in \Sigma$ such that
$$z_n \in \operatorname*{argmin}_{z\in\Sigma} \mathcal{E}\left(u_{n-1} + z\right);$$
3. find $(\beta_1^n, \cdots, \beta_n^n) \in \mathbb{R}^n$ such that
$$(\beta_1^n, \cdots, \beta_n^n) \in \operatorname*{argmin}_{(\beta_1,\cdots,\beta_n)\in\mathbb{R}^n} \mathcal{E}\left(\sum_{k=1}^n \beta_k z_k\right);$$
4. set $u_n = \sum_{k=1}^n \beta_k^n z_k$ and $n = n+1$. Return to step 2.

The same convergence results as for the Pure Greedy algorithm hold for the Orthogonal Greedy algorithm.

More on the quadratic case

Two cases where we know a little more on approximations with rank-1 tensor product functions:

- **The Singular Value Decomposition (SVD) case:** Only two Hilbert spaces V_x and V_y, $\mathcal{E}(v) = \|v-u\|_V^2$ and $\|r \otimes s\|_V = \|r\|_{V_x}\|s\|_{V_y}$.

  Orthogonality relations: $\forall n \neq n',\ \langle r_n, r_{n'}\rangle_{V_x} = \langle s_n, s_{n'}\rangle_{V_y} = 0.$

  Optimal decomposition: at iteration n, $u_n = \sum_{k=1}^n r_k \otimes s_k$ is the minimizer of $\|\sum_{k=1}^n \phi_k \otimes \psi_k - u\|_V^2$ over all possible $(\phi_k, \psi_k)_{1\leq k\leq n} \in (V_x \times V_y)^n$.

- **The linear case:** ([De Vore, Temlyakov, 1996] [Le Bris, TL, Maday, 2009]) Either more than two Hilbert spaces or $\mathcal{E}(v) = \|v-u\|_V^2$ (but $\|r \otimes s\|_V \neq \|r\|_{V_t}\|s\|_{V_x}$)

  Example: $\mathcal{E}(v) = \frac{1}{2}\int_{\Omega_x\times\Omega_y} |\nabla_{x,y} v|^2 - \int_{\Omega_x\times\Omega_y} fv = \|v-u\|^2_{H_0^1(\Omega_x\times\Omega_y)}$ where $-\Delta_{x,t} u = f$.

  The above orthogonality relations do not hold anymore, however, the following convergence rates hold in the infinite dimensional case: there exists $C > 0$ such that for all $n \in \mathbb{N}^*$,
  Pure Greedy Algorithm: $\|u_n - u\|_V \leq Cn^{-1/6}$.
  Orthogonal Greedy Algorithm: $\|u_n - u\|_V \leq Cn^{-1/2}$.

Outline

The tyre problem

Uncertainty quantification on a model of tyre

Complex contact problem!

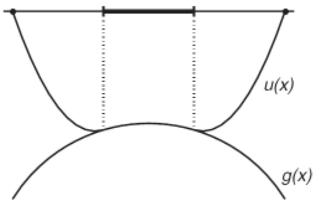
Uncertainty sources:

- Mechanical characteritics of the materials (Young modulus ...)
- Geometrical uncertainties
- Profile of the road

Output of interest:

- $p_0 = \frac{1}{|\Gamma|}\int_\Gamma p$: Mean pressure on Γ the part of the tyre which is in contact with the soil
- $\int_\Gamma |p - p_0|^2$

Rope hanging over an obstacle



T: Random vector modelizing some uncertain parameters in the model.
x: Position
x and T respectively take values in $\mathcal{X}$ and $\mathcal{T}$.

$z(T, x)$: Height of the rope
$g(T, x)$: Height of the obstacle
$f(T, x)$: Stresses applied to the rope

Notation: $L^2_T(\mathcal{T}, H_x) = \left\{ v : \mathcal{T} \to H_x \mid \mathbb{E}\left[\|v(T)\|^2_{H_x} \right] < +\infty \right\}$

$g \in L^2_T(\mathcal{T}, H^1_0(\mathcal{X}))$, $f \in L^2_T(\mathcal{T}, L^2(\mathcal{X}))$.

Rope hanging over an obstacle

Find $z \in L^2(\mathcal{T}, H_0^1(\mathcal{X}))$ such that

$$\left\{ \begin{array}{c} -\Delta_x z \geq f \ \text{ sur } \mathcal{T} \times \mathcal{X}, \\ z \geq g \ \text{ sur } \mathcal{T} \times \mathcal{X}, \\ (\Delta_x z + f)(z - g) = 0 \ \text{ sur } \mathcal{T} \times \mathcal{X}, \\ z(T,x) = 0 \quad \forall (T,x) \in \mathcal{T} \times \partial\mathcal{X}. \end{array} \right.$$

Equivalent formulation:

$$\mathcal{K} = \left\{ v \in L^2(\mathcal{T}, H_0^1(\mathcal{X})) \mid v(T,x) \geq g(T,x) \ \forall (T,x) \in \mathcal{T} \times \mathcal{X} \right\}$$

$$z = \underset{v \in \mathcal{K}}{argmin}\, \mathcal{J}(v)$$

with $\mathcal{J}(v) = \mathbb{E}\left[\frac{1}{2} \int_{\mathcal{X}} |\nabla_x v(T,x)|^2 \, dx - \int_{\mathcal{X}} f(T,x) v(T,x) \, dx \right]$

Penalized formulation

Problem: $\mathcal{K}$ is not a Hilbert space!!

We introduce a series of approached problems: $\rho > 0$ (large)

$$z_\rho = \text{argmin}_{v \in L^2_T(\mathcal{T}, H^1_0(\mathcal{X}))} \mathcal{J}_\rho(v)$$

where $\boxed{\mathcal{J}_\rho(v) = \mathbb{E}\left[\frac{1}{2}\int_{\mathcal{X}} |\nabla_x v(T,x)|^2\,dx - \int_{\mathcal{X}} f(T,x)v(T,x)\,dx + \frac{\rho}{2}\int_{\mathcal{X}} [g(T,x) - v(T,x)]_+^2\,dx\right]}$

$$z_\rho \underset{\rho \to +\infty}{\longrightarrow} z$$

Our aim is to approximate $z_\rho = u$ for a given value of ρ with the greedy algorithm. Let us denote $V = L^2_T(\mathcal{T}, H^1_0(\mathcal{X}))$, $\mathcal{E} = \mathcal{J}_\rho$.

The penalized problem can be rewritten under a more general form:

$$\boxed{u = \underset{v \in V}{\operatorname{argmin}}\, \mathcal{E}(v)}$$

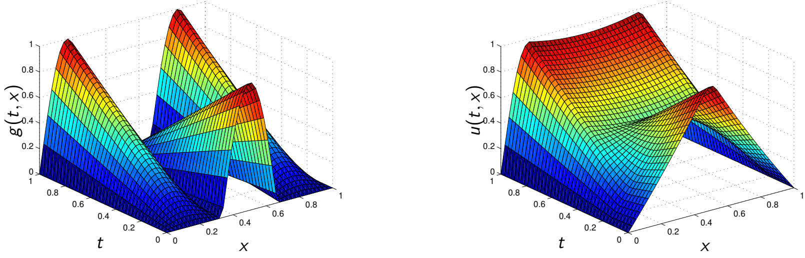
Numerical results

Assumptions (H1), (H2), (H3), (H4) and (H5) are satisfied with $V_t = L^2_T(\mathcal{T})$ and $V_x = H^1_0(\mathcal{X})$ ($V = V_t \otimes V_x$).

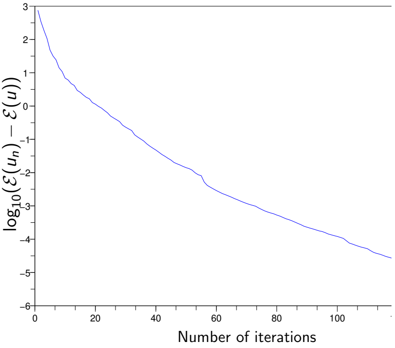
$\mathcal{X} = \mathcal{T} = (0,1)$. T uniform law of probability on $(0,1)$.

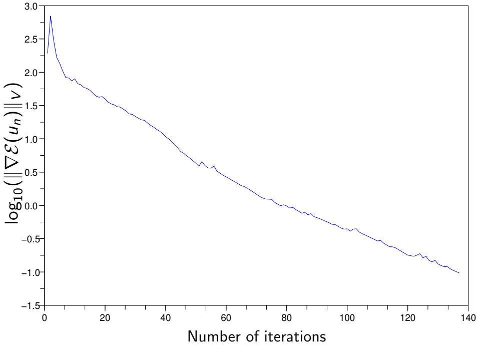
$$f(t,x) = -1 \text{ and } g(t,x) = t[sin(3\pi x)]_+ + (t-1)[sin(3\pi x)]_-.$$

$\rho = 2500$



Rate of convergence





Outline

Conclusions

- Presentation of greedy algorithms in the context of high-dimensionnal convex problems
- Illustration to the study of uncertainty quantification on an obstacle problem via penalization methods on a toy example
- Problems involving a larger number of variables/parameters can also be tackled using this method
- Greedy algorithms can also be used for the resolution of high-dimensional eigenvalue problems (parametric and non-parametric): application to the resolution of the many-body Schrdinger electronic problem (joint work with Eric Cancès, Tony Lelièvre and Majdi Hochlaf)

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Thank you for your attention!

Linear eigenvalue problem

Let V, H be separable Hilbert spaces such that

(V1) $V \subset H$ is dense and the injection $V \hookrightarrow H$ is compact;

and let $a : V \times V \to \mathbb{R}$ be a **continuous symmetric bilinear form** such that

(A1) $\exists \kappa > 0, \nu \in \mathbb{R}, \quad \forall v \in V,\ a(v,v) \geq \kappa \|v\|_V^2 - \nu \|v\|_H^2.$

We wish to compute the lowest eigenvalue μ of the bilinear form a, which satisfies

$$\mu = \inf_{v \in V,\ v \neq 0} \frac{a(v,v)}{\|v\|_H^2}$$

and an associated H-normalized eigenvector $u \in V$, i.e. such that $\|u\|_H = 1$ and

$$\forall v \in V,\ a(u,v) = \mu \langle u, v \rangle_H.$$

$\Sigma \subset V$ satisfying $(\Sigma 1)$, $(\Sigma 2)$ and $(\Sigma 3)$.

$$\lambda_\Sigma := \inf_{z \in \Sigma, z \neq 0} \frac{a(z,z)}{\|z\|_H^2}.$$

Three greedy algorithms

- Rayleigh Greedy algorithm ([Cancès, VE, Lelièvre, 2012]);
- Residual Greedy algorithm ([Cancès, VE, Lelièvre, 2012]);
- Explicit Greedy algorithm ([Chinesta, Ammar, 2010]);

All these algorithms rely on the choice of an initial guess $u_1 \in V$ such that $\|u_1\|_H = 1$.

Rayleigh Greedy algorithm

Rayleigh quotient: $\forall v \in V,\ \mathcal{J}(v) := \begin{cases} \frac{a(v,v)}{\|v\|_H^2} \text{ if } v \neq 0, \\ +\infty \text{ if } v = 0. \end{cases}$

The Rayleigh Greedy algorithm reads:

1. choose $u_1 \in V$ such that $\|u_1\|_H = 1$, set $\lambda_1 := a(u_1, u_1)$ and $n = 2$;
2. find $z_n \in \Sigma$ such that

$$z_n \in \underset{z \in \Sigma}{\operatorname{argmin}}\, \mathcal{J}\left(u_{n-1} + z\right). \tag{3}$$

3. set $u_n = \frac{u_{n-1}+z_n}{\|u_{n-1}+z_n\|_H}$, $\lambda_n := a(u_n, u_n)$ and $n = n + 1$. Return to step 2.

Euler equations associated to (3) when Σ is the set of rank-1 tensor-products (1): $\forall(\delta r, \delta s) \in V_x \times V_y$,

$$(a - \lambda_n)(u_n, r_n \otimes \delta s + \delta r \otimes s_n) = 0.$$

Residual Greedy algorithm

The Residual Greedy algorithm reads:

1. choose $u_1 \in V$ such that $\|u_1\|_H = 1$, set $\lambda_1 := a(u_1, u_1)$ and $n = 2$;
2. find $z_n \in \Sigma$ such that
$$z_n \in \operatorname*{argmin}_{z \in \Sigma} \mathcal{R}_n(z). \quad (4)$$
3. set $u_n = \frac{u_{n-1}+z_n}{\|u_{n-1}+z_n\|_H}$, $\lambda_n := a(u_n, u_n)$ and $n = n+1$. Return to step 2.

where for all $n \in \mathbb{N}^*$ and all $v \in V$,

$$\mathcal{R}_n(v) := \frac{1}{2}(a+\nu)(u_{n-1}+v, u_{n-1}+v) - (\lambda_{n-1}+\nu)\langle u_{n-1}, v\rangle_H.$$

Euler equations associated to (4) when Σ is the set of rank-1 tensor product (1): $\forall(\delta r, \delta s) \in V_x \times V_y$,

$$(a+\nu)(u_n, r_n \otimes \delta s + \delta r \otimes s_n) - (\lambda_{n-1}+\nu)\langle u_{n-1}, r_n \otimes \delta s + \delta r \otimes s_n\rangle_H = 0.$$

Convergence results in infinite dimension

Theorem (Cancès, VE, Lelièvre, 2012)

Provided that (A1), (V1), (Σ1), (Σ2), (Σ3) and that $\lambda_1 \leq \lambda_\Sigma$*, the iterations of the Rayleigh (up to a slight modification) and Residual Greedy algorithms are well-defined. Besides, the sequence* $(\lambda_n)_{n\in\mathbb{N}}$ *converges to* λ*, an eigenvalue of the bilinear form a. Besides, if* F_λ *denotes the set of H-normalized eigenfunctions of a associated with the eigenvalue* λ*,*

$$d(u_n, F_\lambda) := \inf_{w\in F_\lambda} \|u_n - w\|_V \underset{n\to\infty}{\longrightarrow} 0.$$

If the eigenvalue λ *is simple, the sequence* $(u_n)_{n\in\mathbb{N}^*}$ *strongly converges in V towards an element* $w_\lambda \in F_\lambda$ *such that* $\|w_\lambda\|_H = 1$*.*

Unfortunately, λ may not be the smallest eigenvalue of a: this depends strongly on the choice of the initial guess u_1.
In the case when the eigenvalue λ is not simple, the uniqueness of the limit is not guaranteed.

Convergence results in finite dimension for the Residual algorithm

Lojasiewicz inequality: ([Lojasiewicz, 1965], [Levitt, 2012])

Lemma

Let $\mathcal{D} := \{u \in V,\ 1/2 < \|u\| < 3/2\}$. Besides, let F_λ be the set of H-normalized eigenvectors of $a(\cdot,\cdot)$ associated to λ. Then, $\mathcal{J} : \mathcal{D} \to \mathbb{R}$ is analytic, and there exists $K > 0$, $\theta \in (0, 1/2]$ and $\varepsilon > 0$ such that

$$\forall u \in \mathcal{D},\ d(u, F_\lambda) := \inf_{w \in F_\lambda} \|u - w\| \leq \varepsilon,\ |\mathcal{J}(u) - \lambda|^{1-\theta} \leq K \|\nabla \mathcal{J}(u)\|_* . \quad (5)$$

Theorem (Cancès, VE, Lelièvre, 2012)

Let us assume (A1), (V1), (Σ1), (Σ2), (Σ3), $\lambda_1 \leq \lambda_\Sigma$ and that the dimension of V is finite. Then, for the Residual algorithm, the whole sequence $(u_n)_{n\in\mathbb{N}^*}$ strongly converges in V towards an element w_λ of F_λ. Besides, if θ denotes the same real number appearing in (5), the following convergence rates hold:

- *if $\theta = 1/2$, there exists $C > 0$ and $0 < \sigma < 1$ such that for n large enough,*

$$\|u_n - w_\lambda\|_a \leq C\sigma^n; \quad (6)$$

- *if $\theta \neq 1/2$, there exits $C > 0$ such that*

$$\|u_n - w_\lambda\|_a \leq C n^{-\frac{\theta}{1-2\theta}} . \quad (7)$$

Explicit Greedy algorithm

The Explicit Greedy algorithm is not defined for general dictionaries.
For the set of rank-1 tensor-product, at iteration n, the pair $(r_n, s_n) \in V_x \times V_y$ is defined through the "Euler" equation: $\forall (\delta r, \delta s) \in V_x \times V_y$,

$$(a - \lambda_{n-1})(u_n, r_n \otimes \delta s + \delta r \otimes s_n) = 0.$$

No mathematical results on this method, even if it seems very efficient in practice for **scalar** problems. Does not seem to converge for vectorial problems.

Choice of the initial guess

To ensure that $\lambda_1 \leq \lambda_\Sigma$, in all the numerical results presented hereafter, the initial guess is chosen according to the following procedure:

1. find $z_1 \in \Sigma$ such that
$$z_1 \in \operatorname*{argmin}_{z \in \Sigma} \mathcal{J}(z);$$
2. set $u_1 := \frac{z_1}{\|z_1\|_H}$.

Orthogonal versions of the algorithms

[Le Bris, Lelièvre, Maday, 2009], [Nouy, Falco, 2011]

The so-called Orthogonal Greedy algorithm reads:

1. set $u_0 = 0$ and $n = 1$;
2. find $z_n \in \Sigma$ as in the second step of the algorithms (Rayleigh, Residual).
3. find $(\beta_1^n, \cdots, \beta_n^n) \in \mathbb{R}^n$ such that

$$(\beta_1^n, \cdots, \beta_n^n) \in \underset{(\beta_1, \cdots, \beta_n) \in \mathbb{R}^n}{\text{argmin}} \mathcal{J}\left(\sum_{k=1}^n \beta_k z_k \right);$$

4. set $u_n = \frac{\sum_{k=1}^n \beta_k z_k}{\left\| \sum_{k=1}^n \beta_k z_k \right\|_H}$. If $\langle u_n, u_{n-1} \rangle_H \leq 0$, set $u_n = -u_n$. Set $n = n+1$ and return to step 2.

The two previous theorems still hold!

Practical implementation

When Σ is the set of rank-1 tensor product functions (1), a fixed-point procedure is also used to compute $(r_n, s_n) \in V_x \times V_y$ at each iteration $n \in \mathbb{N}^*$.

- Residual and Explicit algorithms: only requires the inversion of small-dimensional linear problems (like in the greedy algorithms for quadratic minimization problems);
- Rayleigh algorithm: requires the full diagonalization of small-dimensional bilinear forms.

Toy numerical tests with matrices

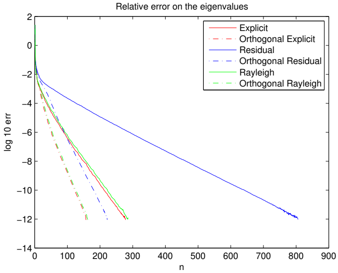
$V := \mathbb{R}^{N_x \times N_y}$, $V_x := \mathbb{R}^{N_x}$, $V_y := \mathbb{R}^{N_y}$, $\Sigma := \left\{ rs^T, \; r \in V_x, \; s \in V_y \right\}$.

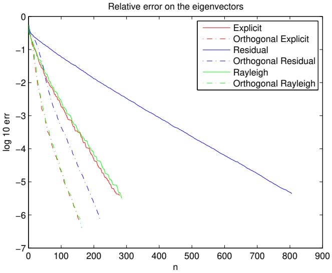
For all $M_1, M_2 \in V$,

$$a(M_1, M_2) := \mathrm{Tr}\left[M_1^T \left(P^x M_2 P^y + Q^x M_2 Q^y \right) \right],$$

with $P^x, Q^x \in \mathbb{R}^{N_x \times N_x}$ and $P^y, Q^y \in \mathbb{R}^{N_y \times N_y}$ symmetric matrices.

Computing the smallest eigenvalue of a is equivalent to computing the smallest eigenvalue of the symmetric matrix
$A = (A_{ij,kl})_{1 \leq i,k \leq N_x, \; 1 \leq j,l \leq N_y} \in \mathbb{R}^{(N_x \times N_y) \times (N_x \times N_y)}$, where $A_{ij,kl} = P^x_{ik} P^y_{jl} + Q^x_{ik} Q^y_{jl}$.





Buckling mode of the microstructured plate

$$V^u := \left\{ \overline{u} = (\overline{u}_x, \overline{u}_y) \in \left(H^1(\Omega_x \times \Omega_y)\right)^2, \ \overline{u}_x = \overline{u}_y = 0 \text{ on } \Gamma_b \right\},$$
$$V^v := \left\{ \overline{v} \in H^2(\Omega_x \times \Omega_y), \ \overline{v} = \nabla \overline{v} \cdot \mathbf{n} = 0 \text{ on } \Gamma_b \cup \Gamma_t \right\}.$$

$$dW^0\left((u^1, v^1), (u^2, v^2)\right) = dW^0_u(u^1, u^2) + dW^0_v(v^1, v^2),$$

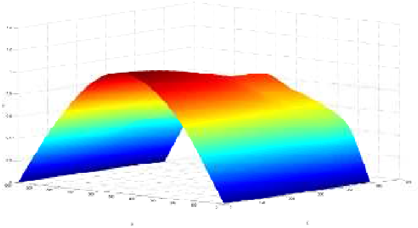
To determine whether there is buckling, we only need to compute the smallest eigenvalue of the bilinear form $a_v := dW^0_v : V^v \times V^v \to \mathbb{R}$.

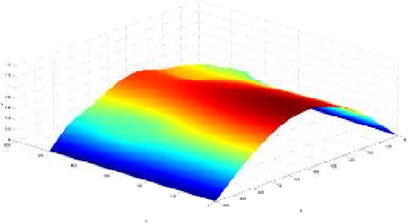
Continuous setting: $\Sigma := \left\{ r \otimes s, r \in V^v_x, \ s \in V^v_y \right\}$ **with**

$$V^v_x := \left\{ r \in H^2(\Omega_x), \ r(0) = r'(0) = r(2) = r'(2) = 0 \right\} \quad \textbf{and} \quad V^v_y := H^2(\Omega_y).$$

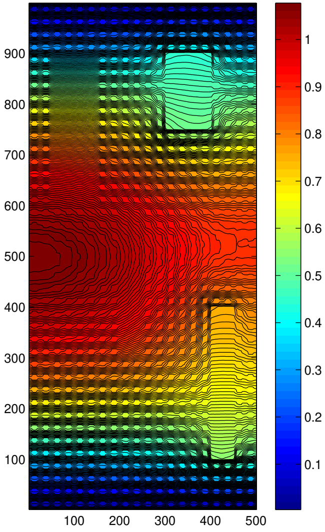
Discrete setting: cubic splines $\otimes$ cubic splines.
The resolution of the full discretized problem via classical galerkin methods would require the computation of the lowest eigenvalue of **one** $10^6 \times 10^6$ matrix!
With the greedy algorithm, we only need the diagonalization (Rayleigh) or the inversion (Residual and Explicit) of **several** matrices whose maximum size is 2000×2000.

Numerical results





Numerical results



Conclusions

- Parametric eigenvalue problems: the eigenvalue is itself a high-dimensional function!
- Electronic structure calculations: theoretical and practical issues
- Nonlinear eigenvalue problems: ex:Gross-Pitaevskii model

$$-\Delta u + u^3 = \mu u.$$

Thank you for your attention!