

Low-rank methods and Proper Generalized Decompositions
—
Application to parametric and stochastic problems

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Stochastic/parametric model

$$u : \Xi \rightarrow \mathcal{V} \quad \text{such that} \quad \mathcal{F}(u(\xi); \xi) = 0$$

where ξ are parameters or random variables taking values in a measure space (Ξ, μ) .

- **Forward problem:**

Given μ , compute a variable of interest

$$s(\xi) = \ell(u(\xi); \xi)$$

and quantities of interest (e.g. statistical moments, probability of events, sensitivity indices)

- **Optimization or inverse problem:**

Given observations of $s(\xi)$, determine ξ or estimate μ .

- $\Xi \subset \mathbb{R}^d$: parameter set
- μ : finite measure on Ξ
- ξ : parameters values or Ξ -valued random variable with probability law μ .
- \mathcal{V} : solution space for the physical model

Uncertainty quantification using functional approaches

Ideal approach

Compute an accurate approximation of $u(\xi)$ (reduced order model, metamodel, surrogate...) that allows fast evaluations of output variables of interest, observables, or objective function.

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Issues

1 Complex numerical models

$$u(\xi) \in \mathcal{V}_{\mathcal{N}}, \quad \mathcal{F}_{\mathcal{N}}(u(\xi); \xi) = 0$$

$$\mathcal{N} \gg 1$$

2 Approximation of multivariate functions

$$u(\xi_1, \dots, \xi_d), \quad (\xi_1, \dots, \xi_d) \in \Xi \subset \mathbb{R}^d$$

$$d \gg 1$$

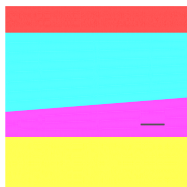
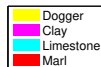
Example: Diffusion in heterogeneous media

Diffusion equation with a random diffusion coefficient κ :

$$-\nabla \cdot (\kappa \nabla u) = f \quad + \quad \text{boundary conditions}$$

- Groundwater flow. Geological layers with uncertain properties:

$$\kappa(x, \omega) = \sum_{i=1}^4 \xi_i(\omega) I_{D_i}(x)$$

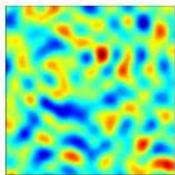
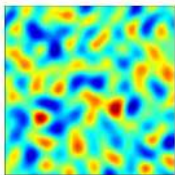
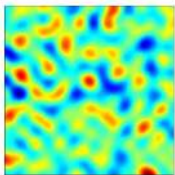


| Layer | Probability Law |
|-------------------|---|
| D_1 : Dogger | $\xi_1 \sim LU(5, 125)$ |
| D_2 : Clay | $\xi_2 \sim LU(3 \cdot 10^{-7}, 3 \cdot 10^{-5})$ |
| D_3 : Limestone | $\xi_3 \sim LU(1.2, 30)$ |
| D_4 : Marl | $\xi_4 \sim LU(10^{-5}, 10^{-4})$ |

$$u(\xi) \in \mathcal{V}_{\mathcal{N}}, \quad \mathcal{N} \gg 1$$

- Random media with spatially correlated random fields

$$\kappa(x, \omega) = \exp(\underline{g}(x) + \sum_{i=1}^d \sqrt{\sigma_i} g_i(x) \xi_i(\omega)), \quad d \gg 1$$



- 1 Model reduction methods for high dimensional problems
- 2 Tensors and tensor-structured problems
- 3 Tensor-structured parametric and stochastic equations
- 4 Low-rank approximation of order-two tensors
- 5 Low-rank methods for parametric and stochastic equations
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High dimensional problems

- Many problems in computational science and engineering require the **approximation of multivariate functions**:

$$u(x_1, \dots, x_d)$$

- Classical discretization methods introduce **high-dimensional parametrizations**

$$u(x_1, \dots, x_d) \approx \sum_{i_1=1}^{n_1} \dots \sum_{i_d=1}^{n_d} a_{i_1 \dots i_d} \varphi_{i_1}^1(x_1) \dots \varphi_{i_d}^1(x_d)$$

$$a \in \mathbb{R}^{n_1 \times \dots \times n_d}$$

- Model order reduction methods aim at **replacing a complex model with a simplified one**, living in a lower dimensional space (or manifold).

- Order reduction methods exploit specific structures (application dependent)

- Smoothness
- Low effective dimensionality, e.g.

$$u(x_1, \dots, x_d) \approx g(x_1, x_2)$$

- Low-order interactions, e.g.

$$u(x_1, \dots, x_d) \approx u_0 + \sum_i u_i(x_i) + \sum_{i \neq j} u_{i,j}(x_i, x_j)$$

- Sparsity (relatively to a basis or frame)
- Low-rank structure

- Structures possibly discovered with suitable parametrizations

$$u(x_1, \dots, x_d) \approx g(y_1, \dots, y_m), \quad (y_1, \dots, y_m) = h(x_1, \dots, x_d),$$

with g smooth, sparse, low-rank, ...

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- Depend on the objectives

- L^∞ optimality (global optimization, inverse problems)
- L^p optimality (energy, moments)
- ...

- Depends on the available information on the function

- Pointwise evaluations

$$u(x_1^k, \dots, x_d^k)$$

- Equations (ODE, PDE, DAE)
- Partial pointwise evaluations (e.g. for parametric/stochastic problems):
equations for

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Low **rank** **tensor** approximation :

What is a **tensor** ?

What is a **tensor**-structured problem ?

What is the **rank** of a tensor ?

Tensor spaces

An algebraic tensor space $V = V_1 \otimes \dots \otimes V_d$ is the set of elements of the form


$$u = \sum_{i=1}^m v_i^1 \otimes \dots \otimes v_i^d$$

or for multivariate functions

$$u(x_1, \dots, x_d) = \sum_{i=1}^m v_i^1(x_1) \dots v_i^d(x_d).$$

A tensor Banach space $V_{\|\cdot\|}$ is obtained by the completion of the algebraic tensor space V with respect to a norm $\|\cdot\|$:

$$V_{\|\cdot\|} = \overline{V_1 \otimes \dots \otimes V_d}^{\|\cdot\|}.$$

 [W. Hackbusch.](#)
Tensor Spaces and Numerical Tensor Calculus,
Springer, 2012.

Examples of (Banach) tensor spaces

- Multidimensional array

$$\begin{aligned}u &\in \mathbb{R}^{n_1 \times \dots \times n_d} = \mathbb{R}^{n_1} \otimes \dots \otimes \mathbb{R}^{n_d} \\u &= \sum_{i_1=1}^{n_1} \dots \sum_{i_d=1}^{n_d} u_{i_1, \dots, i_d} \mathbf{e}_{i_1}^1 \otimes \dots \otimes \mathbf{e}_{i_d}^d\end{aligned}$$

- Finite dimensional tensor spaces:

$$V = V_1 \otimes \dots \otimes V_d = V_{\|\cdot\|}$$

Denoting $\{\phi_i^k\}_{i=1}^{n_k}$ a basis of the n_k -dimensional space V_k , $u \in V$ can be written

$$u = \sum_{i_1=1}^{n_1} \dots \sum_{i_d=1}^{n_d} a_{i_1 \dots i_d} \phi_{i_1}^1 \otimes \dots \otimes \phi_{i_d}^d,$$

and identified with

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Examples of (Banach) tensor spaces

- **Bochner space** $L^p_\mu(\Xi; \mathcal{V})$, the set of Bochner measurable functions u defined on a measure space (Ξ, μ) with values in a Banach space $(\mathcal{V}, \|\cdot\|_{\mathcal{V}})$, with bounded norm

$$\|u\|_p = \left(\int_{\Xi} \|u(\xi)\|_{\mathcal{V}}^p \mu(d\xi) \right)^{1/p} \quad (1 \leq p < \infty),$$

$$\text{or } \|u\|_\infty = \operatorname{ess\,sup}_{\xi \in \Xi} \|u(\xi)\|_{\mathcal{V}} \quad (p = \infty)$$

- An element $u \in L^p_\mu(\Xi) \otimes \mathcal{V}$ is of the form

$$u(\xi) = \sum_{i=1}^m v_i s_i(\xi), \quad \xi \in \Xi.$$

- Case $1 \leq p < \infty$.

$$\overline{L^p_\mu(\Xi) \otimes \mathcal{V}}^{\|\cdot\|_p} = L^p_\mu(\Xi; \mathcal{V})$$

- Case $p = \infty$.

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Examples of (Banach) tensor spaces

- Lebesgue space $L^p_\mu(\Xi)$ with product measure $\mu = \mu_1 \otimes \dots \otimes \mu_d$ on $\Xi = \Xi_1 \times \dots \times \Xi_d$:

$$L^p_\mu(\Xi_1 \times \dots \times \Xi_d) = \overline{L^p_{\mu_1}(\Xi_1) \otimes \dots \otimes L^p_{\mu_d}(\Xi_d)}^{\|\cdot\|_p} \quad (1 \leq p < \infty)$$

An element $u \in L^p_{\mu_1}(\Xi_1) \otimes \dots \otimes L^p_{\mu_d}(\Xi_d)$ is of the form

$$u(\xi_1, \dots, \xi_d) = \sum_{i=1}^m u_i^1(\xi_1) \dots u_i^d(\xi_d), \quad (\xi_1, \dots, \xi_d) \in \Xi.$$

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- **Sobolev space** $W^{s,p}(I)$ on $I = I_1 \times \dots \times I_d$, the set of measurable functions $u : I \rightarrow \mathbb{R}$ with bounded norm

$$\|u\|_{s,p} = \sum_{|\alpha| \leq s} \|\partial^\alpha u\|_p, \quad \partial^\alpha = \partial_1^{\alpha_1} \dots \partial_d^{\alpha_d}.$$

$$W^{s,p}(I) = \overline{W^{s,p}(I_1) \otimes \dots \otimes W^{s,p}(I_d)}^{\|\cdot\|_{s,p}} \quad (1 \leq p < \infty)$$

$W^{s,p}(I)$ is an intersection tensor space:

$$W^{s,p}(I) = \bigcap_{\alpha \in \Lambda_s} \overline{W^{\alpha_1,p} \otimes \dots \otimes W^{\alpha_d,p}}^{\|\cdot\|_\alpha}$$

$$\Lambda_s = \{(0, \dots, 0), (s, 0, \dots, 0), (0, \dots, 0, s)\}$$

- Stochastic/Parametric equations (PDEs, ODEs...):

$$\mathcal{F}(u(\xi); \xi) = 0, \quad u(\xi) \in \mathcal{V}$$

$$\xi \sim \mu, \quad \text{supp}(\mu) = \Xi.$$

$$u \in L_{\mu}^p(\Xi; \mathcal{V}) = \overline{\mathcal{V} \otimes L_{\mu}^p(\Xi)}$$

- Functions of independent random variables:

$$u(\xi_1, \xi_2, \dots, \xi_d)$$

$$\xi_k \sim \mu_k, \quad \text{supp}(\mu_k) = \Xi_k$$

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- Parametrized functions of random variables (robust optimization and control, statistical inverse problems):

$$\begin{aligned}
 & u(\xi, \eta) \\
 & \xi \sim \mu, \quad \text{supp}(\mu) = \Xi, \quad \eta \in A \\
 & u \in \overline{\mathcal{V} \otimes L_{\mu}^p(\Xi) \otimes L_{\nu}^q(A)}
 \end{aligned}$$

- Stochastic calculus:

$$\begin{cases} dX_t = a(X_t, t)dt + \sigma(X_t, t)dW_t \\ X_0 = x_0 \end{cases} \quad X_t = (X_t^1 \dots X_t^n)$$

The probability density function $u(\cdot, t)$ of X_t verifies a n -dimensional PDE (Kolmogorov forward equation)

$$u(\cdot, t) \in \overline{H_{\mu_1}^1(\mathbb{R}) \otimes \dots \otimes H_{\mu_n}^1(\mathbb{R})}$$

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Other tensor structured problems in computational science

- Dynamical systems:

$$\partial_t u(t) = F(u(t); t)$$

$$t \in I, \quad u(t) \in \mathcal{V}$$

$$u \in \overline{H^1(I) \otimes \mathcal{V}}$$

- Multidimensional PDEs

$$\left(\sum_{i,j=1}^d a_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^d b_i \frac{\partial}{\partial x_i} + c \right) u(x_1, \dots, x_d) = f$$

$$(x_1, \dots, x_d) \in \Omega_1 \times \dots \times \Omega_d$$

$$u \in \overline{H^1(\Omega_1) \otimes \dots \otimes H^1(\Omega_d)}$$

- Quantum physics and chemistry (Schrödinger equation, Master equation, ...)
- Problem in a vector space can be made a problem in a tensor space, e.g. through quantization

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Approximation in a subset of tensors with bounded rank

$$\mathcal{M}_{\leq r} = \{v \in V = V_1 \otimes \dots \otimes V_d; \text{rank}(v) \leq r\}$$

- For order-two tensors, a single notion of rank.

$$\begin{aligned} & v \in V_1 \otimes V_2 \\ \text{rank}(v) \leq r & \iff v = \sum_{i=1}^r v_i^1 \otimes v_i^2 \quad \left(v(x_1, x_2) = \sum_{i=1}^r v_i^1(x_1) v_i^2(x_2) \right) \end{aligned}$$

- For higher-order tensors, different notions of rank.

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A class of parametric and stochastic models

$$u(\xi) \in \mathcal{V}, \quad a(u(\xi), w; \xi) = f(w; \xi) \quad \forall w \in \mathcal{W}$$

- Assumption on the parametrized bilinear form $a(\cdot, \cdot; \xi) : \mathcal{V} \times \mathcal{W} \rightarrow \mathbb{R}$

$$\sup_{v \in \mathcal{V}} \sup_{w \in \mathcal{W}} \frac{a(v, w; \xi)}{\|v\|_{\mathcal{V}} \|w\|_{\mathcal{W}}} \leq \gamma(\xi) \leq \bar{\gamma} < \infty$$

$$\inf_{v \in \mathcal{V}} \sup_{w \in \mathcal{W}} \frac{a(v, w; \xi)}{\|v\|_{\mathcal{V}} \|w\|_{\mathcal{W}}} \geq \alpha(\xi) \geq \underline{\alpha} > 0$$

Example 1

$$-\nabla \cdot (\kappa(\cdot, \xi) \nabla u) = g(\cdot, \xi) \quad \text{on } D, \quad u = 0 \quad \text{on } \partial D$$

- $a(u, w; \xi) = \int_D \nabla w(x) \cdot \kappa(x, \xi) \cdot \nabla u(x) \, dx, \quad f(w; \xi) = \int_D g(x, \xi) w(x) \, dx$
- Approximation space $\mathcal{V} \subset H_0^1(D)$, $\mathcal{W} = \mathcal{V}$.
- $\underline{\alpha} \leq \alpha(\xi) \leq \kappa(x, \xi) \leq \gamma(\xi) \leq \bar{\gamma}$

- Corresponding operator equation

$$A(\xi)u(\xi) = f(\xi)$$

$$A(\xi) : \mathcal{V} \rightarrow \mathcal{W}' \quad \text{such that} \quad a(v, w; \xi) = \langle A(\xi)v, w \rangle$$

$$f(\xi) \in \mathcal{W}' \quad \text{such that} \quad f(w; \xi) = \langle f(\xi), w \rangle$$

- Operator $A(\xi)$ is such that

$$\alpha(\xi)\|v\|_{\mathcal{V}} \leq \|A(\xi)v\|_{\mathcal{W}'} \leq \gamma(\xi)\|v\|_{\mathcal{V}}$$

- Given bases $\{\varphi_i\}_{i=1}^{\mathcal{N}}$ and $\{\psi_i\}_{i=1}^{\mathcal{N}}$ of \mathcal{V} and \mathcal{W} , algebraic formulation

$$\mathbf{u}(\xi) \in \mathbb{R}^{\mathcal{N}}, \quad \mathbf{A}(\xi)\mathbf{u}(\xi) = \mathbf{f}(\xi)$$

with $(\mathbf{A}(\xi))_{ij} = \langle A\varphi_j, \psi_i \rangle$, $(\mathbf{f}(\xi))_i = \langle f(\xi), \psi_i \rangle$, and $u(\xi) = \sum_{j=1}^{\mathcal{N}} (\mathbf{u}(\xi))_j \varphi_j$.

- Regularity of the solution

$$\|u(\xi)\|_{\mathcal{V}} \leq \frac{1}{\alpha(\xi)} \|f(\xi)\|_{\mathcal{W}'}$$

If $\alpha(\xi) \geq \underline{\alpha}$ and $f \in L^p_\mu(\Xi; \mathcal{W}')$, then

$$\|u\|_p = \mathbb{E}_\mu(\|u(\xi)\|_{\mathcal{V}}^p)^{1/p} \leq \mathbb{E}_\mu\left(\frac{1}{\alpha(\xi)} \|f(\xi)\|_{\mathcal{W}'}\right)^{1/p} \leq \frac{1}{\underline{\alpha}} \|f\|_p$$

which implies

$$u \in L^p_\mu(\Xi; \mathcal{V}) = \overline{\mathcal{V} \otimes L^p_\mu(\Xi)}^{\|\cdot\|_p}$$

- From now on, assume that

$$u \in L^2_\mu(\Xi; \mathcal{V}) = \overline{\mathcal{V} \otimes L^2_\mu(\Xi)}^{\|\cdot\|_2}$$

Stochastic (or parametric) weak form

Galerkin approximation of the solution in $\overline{\mathcal{V} \otimes L^2_\mu(\Xi)}^{\|\cdot\|_2}$ defined by

$$u \in \mathcal{V} \otimes \mathcal{S}, \quad B(u, w) = F(w) \quad \forall w \in \mathcal{W} \otimes \tilde{\mathcal{S}}$$

- Approximation spaces \mathcal{S} and $\tilde{\mathcal{S}}$ in $L^2_\mu(\Xi)$ (e.g. polynomial chaos). Usually, $\mathcal{S} = \tilde{\mathcal{S}}$ (Parametric Bubnov-Galerkin).

- $B(v, w) = \mathbb{E}_\mu(\langle A(\xi)v(\xi), w(\xi) \rangle) = \int_\Xi \langle A(y)v(y), w(y) \rangle \mu(dy)$

- $F(w) = \mathbb{E}_\mu(\langle f(\xi), w(\xi) \rangle) = \int_\Xi \langle f(y), w(y) \rangle \mu(dy)$

- Corresponding operator equation:

$$Bu = F$$

with $B : \mathcal{V} \otimes \mathcal{S} \rightarrow (\mathcal{W} \otimes \tilde{\mathcal{S}})'$ and $F \in (\mathcal{W} \otimes \tilde{\mathcal{S}})'$ defined by

$$\langle Bu, w \rangle = B(u, w), \quad F(w) = \langle F, w \rangle$$

Tensor structured equations

- Low-rank representations of operator and right-hand side

$$a(v, w; \xi) = \sum_{k=1}^R \lambda_k(\xi) a_k(v, w), \quad A(\xi) = \sum_{k=1}^R \lambda_k(\xi) A_k$$

$$f(\xi) = \sum_{k=1}^L \eta_k(\xi) f_k$$

Example 1

- $\kappa(x, \xi) = \sum_{k=1}^R \lambda_k(\xi) \kappa_k(x), \quad a_k(v, w) = \int_D \nabla w(x) \cdot \kappa_k(x) \cdot \nabla v(x) dx = \langle A_k v, w \rangle$
- $g(\cdot, \xi) = \sum_{k=1}^L \eta_k(\xi) g_k(x), \quad \langle f_k, w \rangle = \int_D g_k(x) w(x) dx$
- If κ and g are not of this form (or if R and L are high), low-rank approximation (e.g. using SVD or Empirical Interpolation method).

Tensor structured equations

- $\lambda : \Xi \rightarrow \mathbb{R}$ can be identified with an operator $\Lambda : \mathcal{S} \rightarrow \tilde{\mathcal{S}}'$ such that

$$\langle \Lambda s, \tilde{s} \rangle = \mathbb{E}_\mu(\lambda(\xi)s(\xi)\tilde{s}(\xi))$$

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- $A(\xi) = \sum_{k=1}^R \lambda_k(\xi)A_k$ defines an operator B from $\mathcal{V} \otimes \mathcal{S}$ to $(\mathcal{W} \otimes \tilde{\mathcal{S}})'$ such that

$$B = \sum_{k=1}^R A_k \otimes \Lambda_k$$

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- Tensor structured equation

$$u \in \mathcal{V} \otimes \mathcal{S}, \quad Bu = F \quad \iff \quad \left(\sum_{k=1}^R A_k \otimes \Lambda_k \right) u = \sum_{k=1}^L f_k \otimes \eta_k$$

- For $\{\Phi_i\}_{i=1}^{\mathcal{P}}$ and $\{\Psi_i\}_{i=1}^{\mathcal{P}}$ bases of \mathcal{S} and $\tilde{\mathcal{S}}$, algebraic representation of Λ :

$$\mathbf{\Lambda} \in \mathbb{R}^{\mathcal{P} \times \mathcal{P}}, \quad (\mathbf{\Lambda})_{ij} = \langle \Lambda \Phi_j, \Psi_i \rangle = \mathbb{E}_{\mu}(\lambda(\xi) \Phi_j(\xi) \Psi_i(\xi))$$

- $u \in \mathcal{V} \otimes \mathcal{S}$ identified with a tensor $\mathbf{u} \in \mathbb{R}^{\mathcal{N}} \otimes \mathbb{R}^{\mathcal{P}}$ such that

$$u = \sum_{i=1}^{\mathcal{N}} \sum_{j=1}^{\mathcal{P}} (\mathbf{u})_{ij} \varphi_i \otimes \Phi_j$$

- Tensor structured equation in algebraic form

$$\mathbf{u} \in \mathbb{R}^{\mathcal{N}} \otimes \mathbb{R}^{\mathcal{P}}, \quad \mathbf{B}\mathbf{u} = \mathbf{F} \quad \iff \quad \left(\sum_{k=1}^R \mathbf{A}_k \otimes \mathbf{\Lambda}_k \right) \mathbf{u} = \sum_{k=1}^L \mathbf{f}_k \otimes \boldsymbol{\eta}_k$$

Higher order tensor structure

- Suppose that $\mu = \mu_1 \otimes \dots \otimes \mu_d$, a product measure on $\Xi_1 \times \dots \times \Xi_d$ (e.g. when $\xi = (\xi_1, \dots, \xi_d)$ are independent random variables). Then

$$L^2_\mu(\Xi) = \overline{L^2_{\mu_1}(\Xi_1) \otimes \dots \otimes L^2_{\mu_d}(\Xi_d)}$$

- Suppose that the approximation space $\mathcal{S} \subset L^2_\mu(\Xi)$ is a finite dimensional tensor space

$$\mathcal{S} = \mathcal{S}_1 \otimes \dots \otimes \mathcal{S}_d, \quad \mathcal{S}_\nu \subset L^2_{\mu_\nu}(\Xi_\nu)$$

and the same for $\tilde{\mathcal{S}} = \tilde{\mathcal{S}}_1 \otimes \dots \otimes \tilde{\mathcal{S}}_d$.

- $\lambda^{(\nu)} : \Xi_\nu \rightarrow \mathbb{R}$ can be identified with an operator $\Lambda^{(\nu)} : \mathcal{S}_\nu \rightarrow \tilde{\mathcal{S}}'_\nu$ such that

$$\langle \Lambda^{(\nu)} s, \tilde{s} \rangle = \mathbb{E}_{\mu_\nu}(\lambda^{(\nu)}(\xi_\nu) s(\xi_\nu) \tilde{s}(\xi_\nu))$$

- A function $\lambda : \Xi \rightarrow \mathbb{R}$ such that $\lambda(\xi) = \lambda^{(1)}(\xi_1) \dots \lambda^{(d)}(\xi_d)$ can be identified with an operator $\Lambda : \mathcal{S} \rightarrow \tilde{\mathcal{S}}'$ such that

$$\Lambda = \Lambda^{(1)} \otimes \dots \otimes \Lambda^{(d)}$$

- Suppose that

$$A(\xi) = \sum_{k=1}^R A_k \lambda_k(\xi), \quad \text{with} \quad \lambda_k(\xi) = \lambda_k^{(1)}(\xi_1) \dots \lambda_k^{(d)}(\xi_d)$$

and

$$f(\xi) = \sum_{k=1}^L f_k \eta_k(\xi), \quad \text{with} \quad \eta_k(\xi) = \eta_k^{(1)}(\xi_1) \dots \eta_k^{(d)}(\xi_d)$$

- Tensor structured equation for $u \in \mathcal{V} \otimes \mathcal{S}_1 \otimes \dots \otimes \mathcal{S}_d$

$$Bu = F \iff \left(\sum_{k=1}^R B_k \otimes \Lambda_k^{(1)} \otimes \dots \otimes \Lambda_k^{(d)} \right) u = \sum_{k=1}^L f_k \otimes \eta_k^{(1)} \otimes \dots \otimes \eta_k^{(d)}$$

- Tensor structured equation in algebraic form for $\mathbf{u} \in \mathbb{R}^{\mathcal{N}} \otimes \mathbb{R}^{\mathcal{P}_1} \otimes \dots \otimes \mathbb{R}^{\mathcal{P}_d}$

$$\mathbf{B}\mathbf{u} = \mathbf{F} \iff \left(\sum_{k=1}^R \mathbf{A}_k \otimes \Lambda_k^{(1)} \otimes \dots \otimes \Lambda_k^{(d)} \right) \mathbf{u} = \sum_{k=1}^L \mathbf{f}_k \otimes \eta_k^{(1)} \otimes \dots \otimes \eta_k^{(d)}$$

- 1 Model reduction methods for high dimensional problems
- 2 Tensors and tensor-structured problems
- 3 Tensor-structured parametric and stochastic equations
- 4 Low-rank approximation of order-two tensors**
- 5 Low-rank methods for parametric and stochastic equations
- 6 Low-rank approximation of higher order tensors
- 7 Higher-order low-rank methods for high-dimensional parametric and stochastic equations

Order-two tensors

- For an order-two tensor $w \in \mathcal{V} \otimes \mathcal{S}$, **single notion of rank**:

$$\text{rank}(w) \leq m \quad \Leftrightarrow \quad w = \sum_{i=1}^m v_i \otimes s_i$$

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$$w(v) = \sum_{i=1}^m s_i \langle v_i, v \rangle, \quad \text{Im}(w) \subset \text{span} \{s_i\}_{i=1}^m$$

The algebraic tensor space $\mathcal{V} \otimes \mathcal{S}$ is identified with the space $\mathcal{F}(\mathcal{V}, \mathcal{S})$ of **finite rank operators** from \mathcal{V} to \mathcal{S} .

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- For $w \in \mathbb{R}^{\mathcal{N}} \otimes \mathbb{R}^{\mathcal{P}}$, $w \in \mathcal{R}_m$ identified with a **rank- m matrix**

$$w = \sum_{i=1}^m v_i \otimes s_i \equiv \sum_{i=1}^m v_i s_i^T \in \mathbb{R}^{\mathcal{N} \times \mathcal{P}}$$

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- $\mathcal{V} \otimes_{\|\cdot\|_{\mathcal{V}}} \mathcal{S}$ equipped with the operator norm $\|\cdot\|_{\mathcal{V}}$ (injective tensor norm) is identified with the closure of $\mathcal{F}(\mathcal{V}, \mathcal{S})$, which is the set of compact operators from \mathcal{V} to \mathcal{S} .

Low-rank approximation of order-two tensors

Consider a tensor

$$u \in \mathcal{V} \otimes_{\|\cdot\|} \mathcal{S}$$

- Rank- m approximation of u

$$u_m = \sum_{i=1}^m v_i \otimes s_i$$

- Best rank- m approximation with respect to $\|\cdot\|$:

$$\|u - u_m\| = \min_{w \in \mathcal{R}_m} \|u - w\|$$

- Best rank- m approximation with respect to a certain “distance” to solution:

$$\mathcal{E}(u, u_m) = \min_{w \in \mathcal{R}_m} \mathcal{E}(u, w)$$

- That defines optimal vectors $\{v_i\}_{i=1}^m$ and $\{s_i\}_{i=1}^m$ with respect to different criteria.

Low-rank approximation of order-two tensors: subspace point of view

- Subspace-based parametrization of \mathcal{R}_m

$$\mathcal{R}_m = \{w \in \mathcal{V}_m \otimes \mathcal{S}_m; \dim(\mathcal{V}_m) = m, \dim(\mathcal{S}_m) = m\}$$

or

$$\mathcal{R}_m = \{w \in \mathcal{V}_m \otimes \mathcal{S}; \dim(\mathcal{V}_m) = m\}$$

- Best rank- m approximation of $u \in \mathcal{V} \otimes \mathcal{S}$

$$\min_{w \in \mathcal{R}_m} \mathcal{E}(u, w) = \min_{\dim(\mathcal{V}_m)=m} \min_{\dim(\mathcal{S}_m)=m} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}_m} \mathcal{E}(u, w)$$

or

$$\min_{w \in \mathcal{R}_m} \mathcal{E}(u, w) = \min_{\dim(\mathcal{V}_m)=m} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}} \mathcal{E}(u, w)$$

- That defines sequences of optimal subspaces \mathcal{V}_m and \mathcal{S}_m (with respect to the chosen "distance"). For $u_m = \sum_{i=1}^m v_i \otimes s_i$, $\mathcal{V}_m = \text{span}\{v_i\}_{i=1}^m$ and $\mathcal{S}_m = \text{span}\{s_i\}_{i=1}^m$.

Hilbert setting: induced norm and SVD

Let \mathcal{V} and \mathcal{S} be Hilbert spaces and $\|\cdot\|$ the canonical (induced) inner product norm,

$$\langle v \otimes s, v' \otimes s' \rangle = \langle v, v' \rangle_{\mathcal{V}} \langle s, s' \rangle_{\mathcal{S}}.$$

- $u \in \mathcal{V} \otimes_{\|\cdot\|} \mathcal{S}$ is identified with an operator $u : v \in \mathcal{V} \rightarrow \langle u, v \rangle_{\mathcal{V}} \in \mathcal{S}$ which is compact and admits a **singular value decomposition**

$$u = \sum_{i=1}^{\infty} \sigma_i v_i \otimes s_i, \quad (\sigma_i) \in \ell_2(\mathbb{N})$$

- The **best rank- m approximation** u_m in the norm $\|\cdot\|$ coincides with the **rank- m truncated singular value decomposition** of u .

$$u_m = \sum_{i=1}^m \sigma_i v_i \otimes s_i$$

- **Notion of decomposition with successive optimality conditions.**
- **Nested subspaces** $\mathcal{V}_m = \text{span}\{v_i\}_{i=1}^m$ and $\mathcal{S}_m = \text{span}\{s_i\}_{i=1}^m$:

$$\mathcal{V}_m \subset \mathcal{V}_{m+1} \quad \text{and} \quad \mathcal{S}_m \subset \mathcal{S}_{m+1}$$

- For $\mathcal{V} = \mathbb{R}^{\mathcal{N}}$ and $\mathcal{S} = \mathbb{R}^{\mathcal{P}}$, the canonical norm $\|\cdot\|$ coincides with the matrix Frobenius norm and

$$u = \sum_{i=1}^{\min(\mathcal{N}, \mathcal{P})} \sigma_i v_i \otimes s_i = V \Sigma S^T$$

with $V \in \mathbb{R}^{\mathcal{N} \times \mathcal{N}}$ and $S \in \mathbb{R}^{\mathcal{P} \times \mathcal{P}}$ orthogonal matrices and $\Sigma \in \mathbb{R}^{\mathcal{N} \times \mathcal{P}}$ a diagonal matrix.

- Natural (induced) norm

$$\|u\|_2 = \left(\int_{\Xi} \|u(\xi)\|_{\mathcal{V}}^2 \mu(d\xi) \right)^{1/2}$$

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- A rank- m approximation u_m is of the form

$$u_m(\xi) = \sum_{i=1}^m v_i s_i(\xi)$$

Low-rank approximation in Bochner Hilbert space $\mathcal{V} \otimes L^2_\mu(\Xi)$

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- The **best rank- r approximation** u_r which solves

$$\min_{v \in \mathcal{R}_m} \|u - v\|_2^2 = \min_{\dim(\mathcal{V}_m)=m} \|u - P_{\mathcal{V}_m} u\|_2^2$$

corresponds to the **truncated singular value decomposition** of $U : L^2_\mu(\Xi) \rightarrow \mathcal{V}$ defined by

$$U\lambda = \int_{\Xi} u(\xi)\lambda(\xi)\mu(d\xi)$$

also known as **Karhunen-Loeve decomposition** for μ a probability measure (or **Proper Orthogonal Decomposition** for ξ the time)

Low-rank approximation in $\mathcal{V} \otimes L_\mu^\infty(\Xi)$

- Let $u \in \mathcal{V} \otimes L_\mu^\infty(\Xi)$, with \mathcal{V} a Hilbert space with inner product $(\cdot, \cdot)_\mathcal{V}$ and norm $\|\cdot\|_\mathcal{V}$.

$$\|u\|_\infty = \operatorname{ess\,sup}_{\xi \in \Xi} \|u(\xi)\|_\mathcal{V}$$

- Optimal rank- m approximation is defined by

$$\min_{v \in \mathcal{R}_m} \|u - v\|_\infty = \min_{\dim(\mathcal{V}_m)=m} \|u - P_{\mathcal{V}_m} u\|_\infty = \min_{\dim(\mathcal{V}_m)} \operatorname{ess\,sup}_{y \in \Xi} \|u(\xi) - P_{\mathcal{V}_m} u(\xi)\|_\mathcal{V}$$

where $P_{\mathcal{V}_m} : \mathcal{V} \rightarrow \mathcal{V}_m$ is the orthogonal projector onto \mathcal{V}_m .

- Set of solutions $\mathcal{K} = \{u(\xi); \xi \in \Xi\} \subset \mathcal{V}$. Assuming \mathcal{K} compact,

$$\min_{v \in \mathcal{R}_m} \|u - v\|_\infty = \min_{\dim(\mathcal{V}_m)=m} \sup_{f \in \mathcal{K}} \|f - P_{\mathcal{V}_m} f\|_\mathcal{V} = d_m(\mathcal{K})_\mathcal{V}$$

where $d_m(\mathcal{K})_\mathcal{V}$ is the Kolmogorov m -width of the set \mathcal{K} .

- In general, optimal spaces are such that

$$\mathcal{V}_m \not\subset \mathcal{V}_{m+1}$$

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- Optimal rank- m approximation is defined by

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Low-rank approximation in $\mathcal{V} \otimes L_\mu^\infty(\Xi)$

- Let $u \in \mathcal{V} \otimes L_\mu^\infty(\Xi)$, with \mathcal{V} a Hilbert space with inner product $(\cdot, \cdot)_\mathcal{V}$ and norm $\|\cdot\|_\mathcal{V}$.

$$\|u\|_\infty = \operatorname{ess\,sup}_{\xi \in \Xi} \|u(\xi)\|_\mathcal{V}$$

- Optimal rank- m approximation is defined by

$$\min_{v \in \mathcal{R}_m} \|u - v\|_\infty = \min_{\dim(\mathcal{V}_m)=m} \|u - P_{\mathcal{V}_m} u\|_\infty = \min_{\dim(\mathcal{V}_m)} \operatorname{ess\,sup}_{y \in \Xi} \|u(\xi) - P_{\mathcal{V}_m} u(\xi)\|_\mathcal{V}$$

where $P_{\mathcal{V}_m} : \mathcal{V} \rightarrow \mathcal{V}_m$ is the orthogonal projector onto \mathcal{V}_m .

- Set of solutions $\mathcal{K} = \{u(\xi); \xi \in \Xi\} \subset \mathcal{V}$. Assuming \mathcal{K} compact,

$$\min_{v \in \mathcal{R}_m} \|u - v\|_\infty = \min_{\dim(\mathcal{V}_m)=m} \sup_{f \in \mathcal{K}} \|f - P_{\mathcal{V}_m} f\|_\mathcal{V} = d_m(\mathcal{K})_\mathcal{V}$$

where $d_m(\mathcal{K})_\mathcal{V}$ is the Kolmogorov m -width of the set \mathcal{K} .

- In general, optimal spaces are such that

$$\mathcal{V}_m \not\subset \mathcal{V}_{m+1}$$

Optimal low-rank approximation in the general case

In the general case (provided well-posedness of minimization problems), best rank- m approximation and corresponding optimal spaces are still well defined by

$$\min_{w \in \mathcal{R}_m} \mathcal{E}(u, w) = \min_{\dim(\mathcal{V}_m)=m} \min_{\dim(\mathcal{S}_m)=m} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}_m} \mathcal{E}(u, w)$$

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BUT

- optimal subspaces are not nested

$$\mathcal{V}_m \not\subset \mathcal{V}_{m+1}, \quad \mathcal{S}_m \not\subset \mathcal{S}_{m+1}$$

- no notion of decomposition

$$u_m = \sum_{i=1}^m v_i^m \otimes s_i^m$$

How to recover a notion of decomposition ?

Suboptimal constructions with nested subspaces and notion of decomposition, based on greedy constructions of the approximation or of subspaces.

- Reduced Basis method (greedy algorithms) and Empirical Interpolation Method (for $L^\infty(\Xi) \otimes \mathcal{V}$)
- Proper Generalized Decompositions (for $L^2(\Xi) \otimes \mathcal{V}$)
- Adaptive Cross Approximation and Empirical Interpolation Method (for $L^\infty \otimes L^\infty$)

Proper Generalized Decomposition

- Greedy construction of the approximation (well-known version of PGD)

Starting from $u_0 = 0$, construction of a sequence $\{u_m\}_{m \geq 1}$ by successive corrections in the "dictionary" of rank-one elements \mathcal{R}_1 :

$$\mathcal{E}(u, u_{m-1} + v_m \otimes s_m) = \min_{w \in \mathcal{R}_1} \mathcal{E}(u, u_{m-1} + w)$$

$$u_m = \sum_{i=1}^m v_i \otimes s_i \in \mathcal{V}_m \otimes \mathcal{S}_m, \quad \mathcal{V}_m = \text{span}\{v_i\}_{i=1}^m, \quad \mathcal{S}_m = \text{span}\{s_i\}_{i=1}^m$$

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- Greedy construction of subspaces (not well known versions of PGD !)

$$\mathcal{E}(u, u_m) = \min_{\substack{\dim(\mathcal{V}_m)=m \\ \mathcal{V}_m \supset \mathcal{V}_{m-1}}} \min_{\substack{\dim(\mathcal{S}_m)=m \\ \mathcal{S}_m \supset \mathcal{S}_{m-1}}} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}_m} \mathcal{E}(u, w) = \min_{v_m \in \mathcal{V}} \min_{s_m \in \mathcal{S}} \min_{\sigma \in \mathbb{R}^{m \times m}} \mathcal{E}(u, \sum_{i,j=1}^m \sigma_{ij} v_i \otimes s_j)$$

or partially greedy construction of subspaces

$$\mathcal{E}(u, u_m) = \min_{\substack{\dim(\mathcal{V}_m)=m \\ \mathcal{V}_m \supset \mathcal{V}_{m-1}}} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}} \mathcal{E}(u, w) = \min_{v_m \in \mathcal{V}} \min_{\{s_j\}_{j=1}^m} \mathcal{E}(u, \sum_{i=1}^m v_i \otimes s_i)$$

- Suboptimal greedy construction of subspaces  [N. 2008; Tamellini, Le Maitre & N. 2013, Giraldi 2012] which are very close to the construction used in Empirical Interpolation Method and Greedy algorithms for Reduced Basis methods.

- Suboptimal greedy construction of subspaces  [N. 2008; Tamellini, Le Maitre & N. 2013, Giraldi 2012] which are very close to the construction used in Empirical Interpolation Method and Greedy algorithms for Reduced Basis methods.
- Suboptimal partial greedy construction of subspaces  [N. 2007]

$$\mathcal{E}(u, u_{m-1} + v_m \otimes s_m) = \min_{v \in \mathcal{V}} \min_{s \in \mathcal{S}} \mathcal{E}(u, u_{m-1} + v \otimes s)$$

$$\mathcal{E}(u, u_m) = \min_{w \in \mathcal{V}_m \otimes \mathcal{S}} \mathcal{E}(u, w), \quad \text{with} \quad \mathcal{V}_m = \text{span}\{v_i\}_{i=1}^m$$

$$u_m = \sum_{i=1}^m v_i \otimes s_i^m$$

Greedy construction of a reduced basis $\{v_1, \dots, v_m, \dots\}$.

Remark : Convergence results are available but still no a priori estimates.

Outline

- 1 Model reduction methods for high dimensional problems
- 2 Tensors and tensor-structured problems
- 3 Tensor-structured parametric and stochastic equations
- 4 Low-rank approximation of order-two tensors
- 5 Low-rank methods for parametric and stochastic equations**
- 6 Low-rank approximation of higher order tensors
- 7 Higher-order low-rank methods for high-dimensional parametric and stochastic equations

Classical iterative methods with low-rank truncations

- Equation in tensor format

$$Bu = F$$

- Iterative solver (Richardson, Gradient...)

$$u^{(k)} = T(u^{(k-1)}) \quad (T: \text{iteration map})$$


For example

$$u^{(k)} = u^{(k-1)} - \alpha(Bu^{(k-1)} - F)$$

- Approximate iterations using low-rank truncations:

$$u^{(k)} \in \mathcal{R}_{m(\epsilon)} \quad \text{such that} \quad \|u^{(k)} - T(u^{(k-1)})\| \leq \epsilon$$

- For the canonical norm $\|\cdot\|$, truncation based on SVD
- Computational requirements: low-rank algebra and efficient SVD algorithms.
- Analysis : perturbation of iterative algorithms.

(see  [Matthies and Zander 2012])

- Tensor structured equation

$$Bu = F$$

- Residual-based error

$$\mathcal{E}(u, w) = \|Bw - F\|_C = \|w - u\|_{B^*CB}$$


with a certain residual norm $\|\cdot\|_C^2 = \langle C\cdot, \cdot \rangle$.

- Best rank- m approximation


$$\mathcal{E}(u, u_m) = \min_{w \in \mathcal{R}_m} \mathcal{E}(u, w)$$

- Assuming $\tilde{\alpha}\|w\| \leq \|w\|_{B^*CB} \leq \tilde{\gamma}\|w\|$, then quasi-optimal approximation:

$$\|u - u_m\| \leq \frac{1}{\tilde{\alpha}} \|Bu_m - F\|_C = \frac{1}{\tilde{\alpha}} \min_{w \in \mathcal{R}_m} \|Bw - F\|_C \leq \frac{\tilde{\gamma}}{\tilde{\alpha}} \min_{w \in \mathcal{R}_m} \|u - w\|$$


- Importance of well-conditioned formulations, with $\frac{\tilde{\gamma}}{\tilde{\alpha}} \approx 1$.
- Construction of preconditioners in low-rank format  [Gibaldi 2012]
- Goal-oriented approach by choosing C such that

$$\|Bw - F\|_C = \|w - u\|_*$$


where $\|\cdot\|_*$ is a norm constructed by taking into account the objective of the computation  [PhD O. Zahm]

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Remark: another residual-based error

$$\mathcal{E}(u, w)^2 = \mathbb{E}_\mu(\|A(\xi)w(\xi) - f(\xi)\|_{D(\xi)}^2) = \mathbb{E}_\mu(\|w(\xi) - u(\xi)\|_{A(\xi)^*D(\xi)A(\xi)}^2)$$

with a certain residual norm $\|\cdot\|_{D(\xi)}$ on \mathcal{W}' . For symmetric problems and $D(\xi) = A(\xi)^{-1}$, it yields $\mathcal{E}(u, w) = \|Bw - F\|_{B^{-1}}$.

- Ideal rank- m approximation u_m defined by

$$\mathcal{E}(u, u_m) = \min_{w \in \mathcal{R}_m} \mathcal{E}(u, w) = \min_{\substack{\dim(\mathcal{V}_m)=m \\ \mathcal{V}_m \supset \mathcal{V}_{m-1}}} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}} \mathcal{E}(u, w)$$

- **Supoptimal greedy construction of subspaces \mathcal{V}_m** : Starting from $\mathcal{V}_0 = 0$, we define a sequence of rank- m approximations u_m by

$$\mathcal{E}(u, u_m) = \min_{\substack{\dim(\mathcal{V}_m)=m \\ \mathcal{V}_m \supset \mathcal{V}_{m-1}}} \min_{w \in \mathcal{V}_m \otimes \mathcal{S}} \mathcal{E}(u, w)$$

Denoting $u_m = \sum_{i=1}^m v_i \otimes s_i^m$, we have

$$\mathcal{E}(u, \sum_{i=1}^m v_i \otimes s_i^m) = \min_{v_m \in \mathcal{V}} \min_{(s_1, \dots, s_m) \in \mathcal{S}^m} \mathcal{E}(u, \sum_{i=1}^m v_i \otimes s_i) \quad (1)$$

- Alternating minimization algorithm for solving (1): solve successively

$$\min_{v_m \in \mathcal{V}} \mathcal{E}(u, \sum_{i=1}^m v_i \otimes s_i)^2, \quad (2)$$

$$\min_{(s_1, \dots, s_m) \in \mathcal{S}^m} \mathcal{E}(u, \sum_{i=1}^m v_i \otimes s_i)^2 \quad (3)$$

- Consider a symmetric problem, and let $C = B^{-1}$ so that

$$\mathcal{E}(u, w)^2 = \|Bw - F\|_{B^{-1}}^2 = \langle Bw - F, w - u \rangle = \mathbb{E}_\mu (\langle A(\xi)w(\xi) - f(\xi), w(\xi) - u(\xi) \rangle)$$

- Solution of (2) (non parametric problem):

$$\min_{\mathbf{v}_m \in \mathcal{V}} \left\| B \sum_{i=1}^m \mathbf{v}_i \otimes \mathbf{s}_i - \mathbf{F} \right\|_{B^{-1}}^2 \Leftrightarrow \left\langle B \sum_{i=1}^m \mathbf{v}_i \otimes \mathbf{s}_i - \mathbf{F}, \tilde{\mathbf{v}} \otimes \mathbf{s}_m \right\rangle = 0 \quad \forall \tilde{\mathbf{v}} \in \mathcal{V}$$

which yields

$$\hat{\mathbf{A}}_{mm} \mathbf{v}_m = \hat{\mathbf{f}}_m - \sum_{i=1}^{m-1} \hat{\mathbf{A}}_{mi} \mathbf{v}_i$$

with

$$\hat{\mathbf{A}}_{mi} = \mathbb{E}_{\mu}(A(\xi) \mathbf{s}_m(\xi) \mathbf{s}_i(\xi)) = \sum_{k=1}^R A_k \hat{\lambda}_{k,m,i}, \quad \hat{\lambda}_{k,m,i} = \mathbb{E}_{\mu}(\lambda_k(\xi) \mathbf{s}_m(\xi) \mathbf{s}_i(\xi))$$

$$\hat{\mathbf{f}}_m = \mathbb{E}_{\mu}(f(\xi) \mathbf{s}_m(\xi)) = \sum_{k=1}^L f_k \hat{\eta}_{k,m}, \quad \hat{\eta}_{k,m} = \mathbb{E}_{\mu}(\eta_k(\xi) \mathbf{s}_m(\xi))$$

- $\hat{\mathbf{A}}_{mi}$ is an evaluation of $A(\xi) = \sum_{k=1}^R A_k \lambda_k(\xi)$ for particular values of the λ_k .
- $\hat{\mathbf{f}}_m$ is an evaluation of $f(\xi) = \sum_{k=1}^L f_k \eta_k(\xi)$ for particular values of the η_k .
- It looks like a sampling approach but it is not ! (no sampling of ξ)

Example 1

$$\langle A(\xi)v, w \rangle = \int_D \nabla w(x) \cdot \kappa(x, \xi) \cdot \nabla v(x) dx, \quad \langle f(\xi), w \rangle = \int_D g(x, \xi) w(x) dx$$

- $\langle \widehat{A}_{mi}v, w \rangle = \int_D \nabla w(x) \cdot \widehat{\kappa}_{mi} \cdot \nabla v(x) dx$ with $\widehat{\kappa}_{mi}(x) = \mathbb{E}_\mu(\kappa(x, \xi) s_m(\xi) s_i(\xi))$
- $\langle \widehat{f}_m, w \rangle = \int_D \widehat{g}_m(x) w(x) dx$ with $\widehat{g}_m(x) = \mathbb{E}_\mu(g(x, \xi) s_m(\xi))$

- Solution of (3) (reduced order parametric problem):

$$\min_{(s_1, \dots, s_m) \in \mathcal{S}^m} \left\| B \sum_{i=1}^m v_i \otimes s_i - F \right\|_{B^{-1}}^2$$

Denoting $\mathbf{s} = (s_i)_{i=1}^m \in (\mathcal{S})^m$, it yields

$$\mathbb{E}_\mu(\mathbf{t}(\xi)^T \mathbf{A}_m(\xi) \mathbf{s}(\xi)) = \mathbb{E}_\mu(\mathbf{t}(\xi)^T \mathbf{f}_m(\xi)) \quad \forall \mathbf{t} \in (\mathcal{S})^m \quad (4)$$

with reduced parametrized matrix and vector

$$(\mathbf{A}_m(\xi))_{ij} = \langle A(\xi) v_j, v_i \rangle, \quad (\mathbf{f}_m(\xi))_i = \langle f(\xi), v_i \rangle.$$

Solution $\mathbf{s}(\xi)$ of (4) is the stochastic Galerkin approximation of the solution of

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- Using low-rank (affine) representations of $A(\xi)$ and $f(\xi)$, we obtain

$$\mathbf{A}_m(\xi) = \sum_{k=1}^R \mathbf{A}_{m,k} \lambda_k(\xi), \quad \mathbf{f}_m(\xi) = \sum_{k=1}^L \mathbf{f}_{m,k} \eta_k(\xi).$$

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- (4) is a system of $m \times \dim(\mathcal{S})$ equations. If $\dim(\mathcal{S}) \gg 1$, structured approximation in \mathcal{S} can be used to reduced the cost (sparsity, low-rank...).

- Solution of (3) (reduced order parametric problem):

$$\min_{(s_1, \dots, s_m) \in \mathcal{S}^m} \left\| B \sum_{i=1}^m v_i \otimes s_i - F \right\|_{B^{-1}}^2$$

Denoting $\mathbf{s} = (s_i)_{i=1}^m \in (\mathcal{S})^m$, it yields

$$\mathbb{E}_\mu(\mathbf{t}(\xi)^T \mathbf{A}_m(\xi) \mathbf{s}(\xi)) = \mathbb{E}_\mu(\mathbf{t}(\xi)^T \mathbf{f}_m(\xi)) \quad \forall \mathbf{t} \in (\mathcal{S})^m \quad (4)$$

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- (4) is a system of $m \times \dim(\mathcal{S})$ equations. If $\dim(\mathcal{S}) \gg 1$, structured approximation in \mathcal{S} can be used to reduced the cost (sparsity, low-rank...).
- (5) can be solved with sampling-based approaches (interpolation, regularized least-squares...)

Example: stochastic Groundwater flow equation (MOMAS/Couplex)

Groundwater flow equation (hydraulic head u)

$$-\nabla(\kappa(x, \xi)\nabla u) = 0 \quad x \in \Omega, \xi \in \Xi$$

+ boundary conditions

Geological layers with uncertain properties



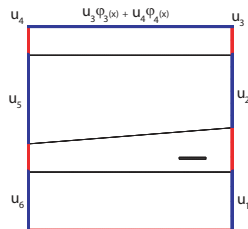
κ 's probability laws

| Layer | Law |
|-----------|--|
| Dogger | $LU(5, 125)$ |
| Clay | $LU(3 \cdot 10^{-7}, 3 \cdot 10^{-5})$ |
| Limestone | $LU(1.2, 30)$ |
| Marl | $LU(10^{-5}, 10^{-4})$ |

10 basic uniform random variables ξ ,

$$\Xi = (-1, 1)^{10}, \text{ uniform probability } P_\xi$$

Uncertain BCs



Neumann homogeneous

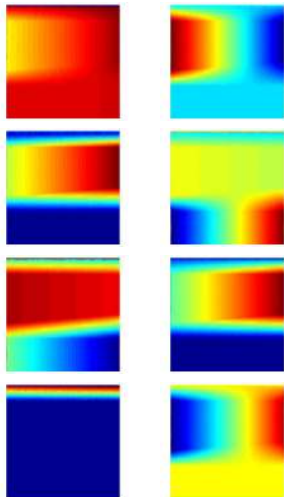
Dirichlet

Law

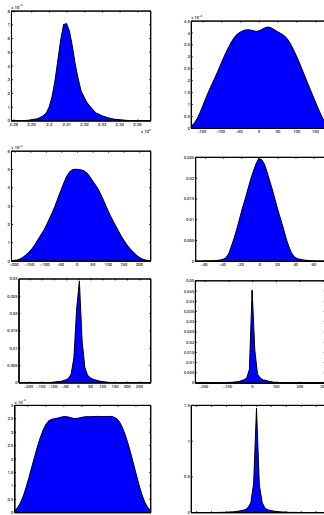
| | |
|-------|---------------|
| u_1 | $U(288, 290)$ |
| u_2 | $U(305, 315)$ |
| u_3 | $U(330, 350)$ |
| u_4 | $U(170, 190)$ |
| u_5 | $U(195, 205)$ |
| u_6 | $U(285, 287)$ |

First modes with the greedy construction of the approximation

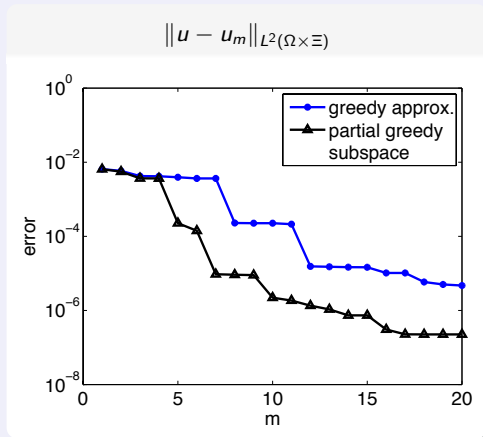
Spatial modes $\{v_1, \dots, v_8\}$



Stochastic modes $\{s_1, \dots, s_8\}$: pdf



Convergence of the progressive PGD (L^2 -norm)



PGD based on Galerkin orthogonality criteria

- Approximation u_m in a subset \mathcal{M}_m
- For symmetric problems

$$\|Bu_m - F\|_{B^{-1}}^2 = \min_{w \in \mathcal{M}_m} \|Bw - F\|_{B^{-1}}^2 = \min_{w \in \mathcal{M}_m} \langle Bw - F, w - u \rangle$$

Necessary (but not sufficient) condition of optimality

$$\langle Bu_m - F, \delta w \rangle = 0 \quad \forall \delta w \in T_{u_m} \mathcal{M}_m \quad (6)$$

where $T_{u_m} \mathcal{M}_m$ is the tangent space to \mathcal{M}_m at u_m .

- For more general problems (provided $B : \mathcal{V} \otimes \mathcal{S} \rightarrow (\mathcal{V} \otimes \mathcal{S})'$), search u_m in \mathcal{M}_m such that it verifies (6).
- Heuristic approach. No theoretical results except for particular cases.

- For the greedy construction of the approximation

$$\mathcal{M}_m = \mathbf{u}_{m-1} + \mathcal{R}_1, \quad \mathbf{u}_m = \mathbf{u}_{m-1} + \mathbf{v}_m \otimes \mathbf{s}_m,$$

$$T_{\mathbf{u}_m} \mathcal{M}_m = T_{\mathbf{v}_m \otimes \mathbf{s}_m} \mathcal{R}_1 = \{\delta \mathbf{v} \otimes \mathbf{s}_m + \mathbf{v}_m \otimes \delta \mathbf{s} : \delta \mathbf{v} \in \mathcal{V}, \delta \mathbf{s} \in \mathcal{S}\}$$

$$(6) \iff \langle B(\mathbf{u}_{m-1} + \mathbf{v}_m \otimes \mathbf{s}_m) - \mathbf{F}, \delta \mathbf{v} \otimes \mathbf{s}_m + \mathbf{v}_m \otimes \delta \mathbf{s} \rangle = 0 \quad \forall \delta \mathbf{v} \in \mathcal{V}, \forall \delta \mathbf{s} \in \mathcal{S}$$

- For the greedy construction of the approximation

$$\mathcal{M}_m = u_{m-1} + \mathcal{R}_1, \quad u_m = u_{m-1} + v_m \otimes s_m,$$

$$T_{u_m} \mathcal{M}_m = T_{v_m \otimes s_m} \mathcal{R}_1 = \{ \delta v \otimes s_m + v_m \otimes \delta s : \delta v \in \mathcal{V}, \delta s \in \mathcal{S} \}$$

$$(6) \iff \langle B(u_{m-1} + v_m \otimes s_m) - F, \delta v \otimes s_m + v_m \otimes \delta s \rangle = 0 \quad \forall \delta v \in \mathcal{V}, \forall \delta s \in \mathcal{S}$$

- For the partial greedy construction of subspaces

$$\mathcal{M}_m = \{ w \in \mathcal{V}_m \otimes \mathcal{S} : \dim(\mathcal{V}_m) = m, \mathcal{V}_m \supset \mathcal{V}_{m-1} \}$$

$$= \left\{ w = \sum_{i=1}^m v_i \otimes s_i : v_m \in \mathcal{V}, \{s_i\}_{i=1}^m \in \mathcal{S}^m \right\}$$

$$T_{u_m} \mathcal{M}_m = \left\{ \delta v \otimes s_m + \sum_{i=1}^m v_i \otimes \delta s_i : \delta v_m \in \mathcal{V}, \{ \delta s_i \}_{i=1}^m \in \mathcal{S}^m \right\}$$

$$(6) \iff \langle B u_m - F, \delta v \otimes s_m + \sum_{i=1}^m v_i \otimes \delta s_i \rangle = 0 \quad \forall \delta v \in \mathcal{V}, \forall \{ \delta s_i \}_{i=1}^m \in \mathcal{S}^m$$

- Use of **alternating direction algorithms**. Computational aspects are similar to the case of symmetric problems described before.
 - **non-parametric problems** of the form

$$\widehat{A}_{mm} v_m = \widehat{f}_m - \sum_{i=1}^{m-1} \widehat{A}_{mi} v_i$$

with

$$\widehat{A}_{mi} = \mathbb{E}_\mu(A(\xi) s_m(\xi) s_i(\xi)) = \sum_{k=1}^R A_k \widehat{\lambda}_{k,m,i}, \quad \widehat{\lambda}_{k,m,i} = \mathbb{E}_\mu(\lambda_k(\xi) s_m(\xi) s_i(\xi))$$

$$\widehat{f}_m = \mathbb{E}_\mu(f(\xi) s_m(\xi)) = \sum_{k=1}^L f_k \widehat{\eta}_{k,m}, \quad \widehat{\eta}_{k,m} = \mathbb{E}_\mu(\eta_k(\xi) s_m(\xi))$$

- **reduced order parametric problems** of the form

$$\mathbf{A}_m(\xi) \mathbf{s}(\xi) = \mathbf{f}_m(\xi) \quad \text{or} \quad a_m(\xi) s_m(\xi) = g_m(\xi) - \sum_{i=1}^{m-1} a_{mi}(\xi) s_i(\xi)$$

- Possible application (heuristic approach) for nonlinear problems. B is a nonlinear map.

Cooling of electronic components

$$-\nabla(\kappa \cdot \nabla u) + DV \cdot \nabla u = f$$

- $\xi_1 = \kappa_{IC} \sim \log \mathcal{U}(0.2, 2) \rightsquigarrow$ diffusion coefficient
- $\xi_2 = r \sim \log \mathcal{U}(0.1, 100) \rightsquigarrow$ thermal contact conductance
- $\xi_3 = D \sim \log \mathcal{U}(5 \cdot 10^{-4}, 10^{-2}) \rightsquigarrow$ advection field

Quantity of interest :

$$S_{\kappa_{IC}} = \frac{\mathbb{V} \left(\mathbb{E} \left(\int_{\Omega_{IC}} u | \kappa_{IC} \right) \right)}{\mathbb{V} \left(\int_{\Omega_{IC}} u \right)}$$

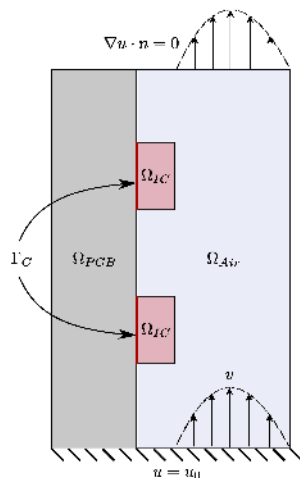


Figure : Geometry

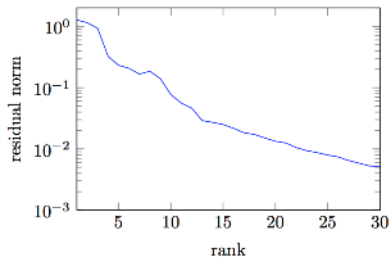


Figure : Evolution of the residual norm

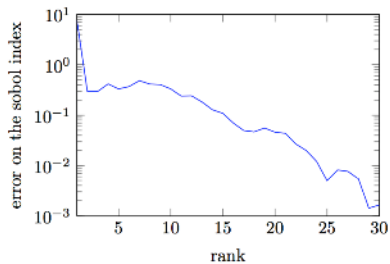
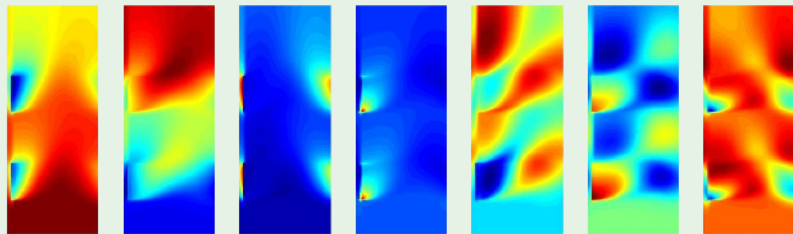


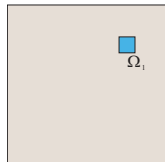
Figure : Error on the Sobol index

First spatial functions v_1 to v_7



Application to an advection-diffusion-reaction equation

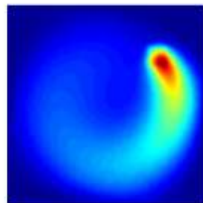
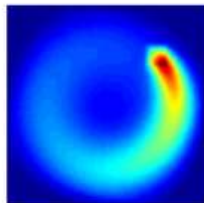
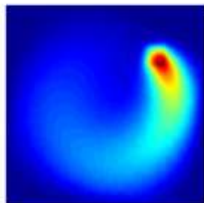
- $\partial_t u - a_1 \Delta u + a_2 c \cdot \nabla u + a_3 u = a_4 I_{\Omega_1}$ on $\Omega \times (0, T)$
- $u = 0$ on $\Omega \times \{0\}$
- $u = 0$ on $\partial\Omega \times (0, T)$



Uncertain parameters

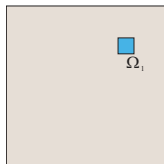
$$a_i(\xi) = \mu_{a_i}(1 + 0.2\xi_i), \quad \xi_i \in U(-1, 1), \quad \Xi = (-1, 1)^4$$

Three samples of the solution $u(x, t, \xi)$



Application to an advection-diffusion-reaction equation

- $\partial_t u - a_1 \Delta u + a_2 c \cdot \nabla u + a_3 u = a_4 I_{\Omega_1}$ on $\Omega \times (0, T)$
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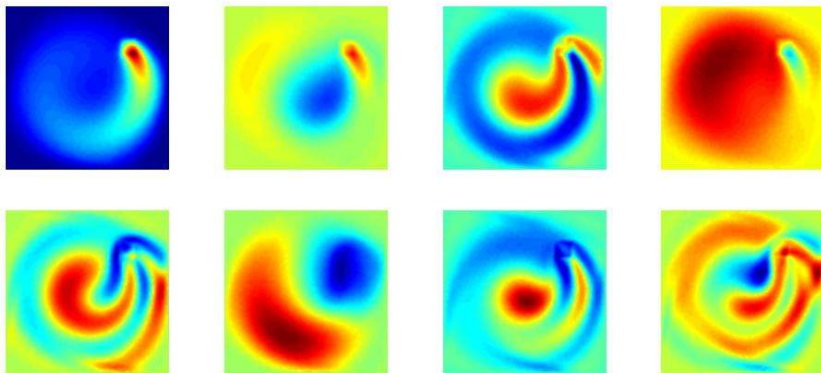
Low-rank approximation of the solution

$$u(x, t, \xi) \approx \sum_{i=1}^m v_i(x, t) s_i(\xi)$$

- Galerkin framework using Time-Discontinuous Galerkin approximation.
- Partial greedy construction of subspaces : Arnoldi-type algorithm  [N. 2008]

Partial greedy construction of subspaces \mathcal{V}_m with Arnoldi-type construction

8 first modes of the decomposition $\{v_1(x, t) \dots v_8(x, t)\}$



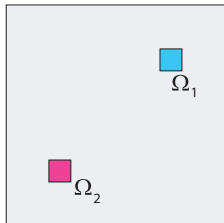
To compute these modes \Rightarrow **only 8 deterministic problems**

Convergence of quantities of interest

Probability density function

Quantity of interest

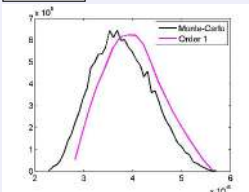
$$s(\xi) = \int_0^T \int_{\Omega_2} u(x, t, \xi) dx dt$$



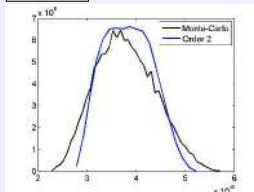
$$s_m(\xi) = \int_0^T \int_{\Omega_2} u_m(x, t, \xi) dx dt$$

Probability density function of $s_m(\xi)$

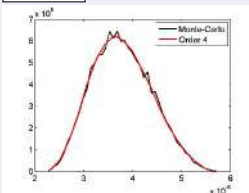
$m = 1$



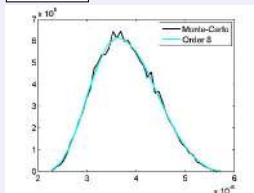
$m = 2$



$m = 4$



$m = 8$

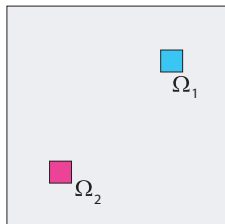


Convergence of quantities of interest

Quantiles

Quantity of interest

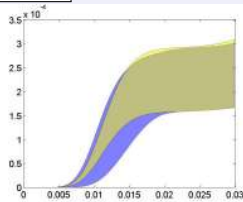
$$s(t, \xi) = \int_{\Omega_2} u(x, t, \xi) dx$$



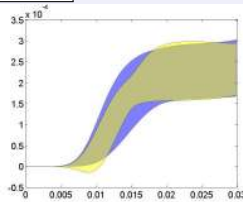
$$s_m(t, \xi) = \int_{\Omega_2} u_m(x, t, \xi) dx$$

99% Quantiles of $s_m(t, \xi)$

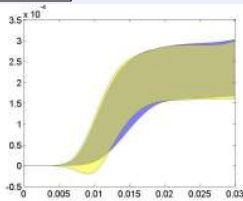
$m = 1$



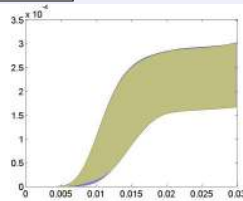
$m = 2$



$m = 4$



$m = 8$



Low-rank approximation using sampling-based approach

- We want to compute an approximation of the solution $u(\xi)$, and then a variable of interest $s(u(\xi); \xi)$, for a collection of samples

$$\{\xi^k\}_{k=1}^K = \Xi_K$$

- The computation of

$$u(\xi^k) = B(\xi^k)^{-1} f(\xi^k) \quad \text{for all } k = 1, \dots, K$$

is unaffordable.

- Use of low-rank approximations ?

Low-rank approximation using sampling-based approach

- For samples $\{\xi^k\}_{k=1}^K = \Xi_K \subset \Xi$, we introduce the **sample-based semi-norm**

$$\|u\|_{2,K} = \left(K^{-1} \sum_{k=1}^K \|u(\xi^k)\|_{\mathcal{V}}^2 \right)^{1/2}$$

- The **best rank- m approximation** u_m which solves

$$\min_{w \in \mathcal{R}_m} \|u - w\|_{2,K}^2 = \min_{w \in \mathcal{R}_m} \frac{1}{K} \sum_{k=1}^K \|u(\xi^k) - w(\xi^k)\|_{\mathcal{V}}^2$$

corresponds to the **truncated singular value decomposition** of the tensor

$$\mathbf{u} = \{u(\xi^k)\}_{k=1}^K \in \mathcal{V}^K = \mathcal{V} \otimes \mathbb{R}^K$$

also known as **Empirical Karhunen-Loeve decomposition**.

- Requires the solution of K independent problems (**Black box simulations**)

$$u(\xi^k) = B(\xi^k)^{-1} f(\xi^k), \quad k = 1, \dots, K$$

Low-rank approximation using sampling-based approach

- Residual based error

$$\mathcal{E}(u, w)^2 = \frac{1}{K} \sum_{k=1}^K \|A(\xi^k)w(\xi^k) - f(\xi^k)\|_{D(\xi^k)}^2 = \|w - u\|_{\tilde{A}, 2, K}^2$$

- Best rank- m approximation defined by

$$\mathcal{E}(u, u_m) = \min_{w \in \mathcal{R}_m} \mathcal{E}(u, w)$$

- The restriction of $u : \Xi \rightarrow \mathcal{V}$ to Ξ_K is identified with the tensor

$$\mathbf{u} = \{u(\xi^k)\}_{k=1}^K \in (\mathcal{V})^K = \mathcal{V} \otimes \mathbb{R}^K$$

- $\|\cdot\|_{\tilde{A}, 2, K}^2$ defines on $\mathcal{V} \otimes \mathbb{R}^K$ a norm which is equivalent to $\|\cdot\|_{2, K}$ and

$$\|u - u_m\|_{2, K} \leq \frac{\tilde{\gamma}}{\tilde{\alpha}} \min_{v \in \mathcal{R}_m} \|u - v\|_{2, K}$$

- Denoting $\hat{\mathbb{E}}_{\mu}^K(f(\xi)) = \frac{1}{K} \sum_{k=1}^K f(\xi^k)$,

$$\mathcal{E}(u, w)^2 = \hat{\mathbb{E}}_{\mu}^K \left(\|A(\xi)w(\xi) - f(\xi)\|_{D(\xi)}^2 \right)$$

- Low-rank algorithms follow the same lines simply replacing $\mathbb{E}_{\mu}(\cdot)$ by $\hat{\mathbb{E}}_{\mu}^K(\cdot)$.

- 1 Model reduction methods for high dimensional problems
- 2 Tensors and tensor-structured problems
- 3 Tensor-structured parametric and stochastic equations
- 4 Low-rank approximation of order-two tensors
- 5 Low-rank methods for parametric and stochastic equations
- 6 Low-rank approximation of higher order tensors**
- 7 Higher-order low-rank methods for high-dimensional parametric and stochastic equations

Approximation of a high-order tensor

$$u \in \overline{V_1 \otimes \dots \otimes V_d}$$

in a subset of low-rank tensors

$$\mathcal{M}_{\leq r} = \{v \in V_1 \otimes \dots \otimes V_d : \text{rank}(v) \leq r\}$$

Rank of higher-order tensors ?

- Canonical rank:

$$\text{rank}(v) \leq r \iff v = \sum_{i=1}^r v_i^1 \otimes \dots \otimes v_i^d \quad \text{or} \quad v(x) = \sum_{i=1}^r v_i^1(x_1) \dots v_i^d(x_d)$$

Parametrization with $\sum_{\nu=1}^d \dim(V_\nu) = O(d)$ parameters.

Example

Ishigami function

$$v(x_1, x_2, x_3) = \sin(x_1) + a \sin(x_2)^2 + bx_3^4 \sin(x_1) = \sin(x_1)(1 + bx_3^4) + a \sin(x_2)^2$$

has a canonical rank 2.

Sparse tensor approximation

Suppose $\{\phi_i^{\nu}(x_{\nu}) : i \in \Lambda_{\nu}\}$ is a basis of V_{ν} (e.g. polynomial spaces). Then

$$\{\phi_{i_1}^1(x_1) \dots \phi_{i_d}^d(x_d) : (i_1, \dots, i_d) \in \Lambda = \Lambda_1 \times \dots \times \Lambda_d\}$$

is a basis of $V_1 \otimes \dots \otimes V_d$. An element $v \in V_1 \otimes \dots \otimes V_d$ can be written

$$v(x_1, \dots, x_d) = \sum_{i \in \Lambda} a_i \phi_{i_1}^1(x_1) \dots \phi_{i_d}^d(x_d)$$

A sparse tensor approximation v_N of v is under the form

$$v_N(x_1, \dots, x_d) = \sum_{i \in \Lambda_N} a_i \phi_{i_1}^1(x_1) \dots \phi_{i_d}^d(x_d)$$

with

$$\Lambda_N \subset \Lambda, \quad \#\Lambda_N = N \ll \#\Lambda$$

and has a canonical rank

$$\text{rank}(v_N) \leq N$$

Consequence: if the best N -term approximation v_N (for a fixed basis) is such that $\|v - v_N\| = \sigma_N$, then

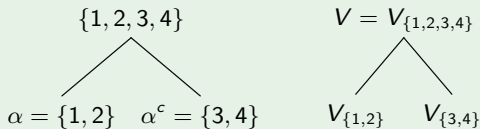
$$\inf_{v_N \in \mathcal{R}_N} \|v - v_N\| \leq \sigma_N$$

- α -rank:

for $\alpha \subset \{1, \dots, d\}$, $V = V_\alpha \otimes V_{\alpha^c}$, with $V_\alpha = \bigotimes_{\mu \in \alpha} V_\mu$ and define the α -rank:

$$\text{rank}_\alpha(v) \leq r_\alpha \iff v = \sum_{i=1}^{r_\alpha} v_i^\alpha \otimes v_i^{\alpha^c}, \quad v_i^\alpha \in V_\alpha, \quad v_i^{\alpha^c} \in V_{\alpha^c}$$

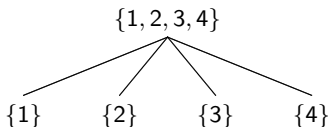
Example



$u(x_1, \dots, x_4) = f(x_1, x_2)g(x_3, x_4)$ is such that $\text{rank}_{(1,2)}(u) = \text{rank}_{(3,4)}(u) = 1$.

- Tucker rank:

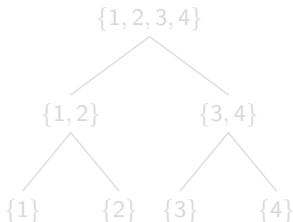
$$\text{rank}_T(v) = (\text{rank}_1(v), \dots, \text{rank}_d(v))$$



$$\text{rank}_T(v) \leq r = (r_1, \dots, r_d) \iff v = \sum_{i_1=1}^{r_1} \dots \sum_{i_d=1}^{r_d} a_{i_1 \dots i_d} v_{i_1}^1 \otimes \dots \otimes v_{i_d}^d$$

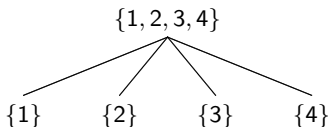
- Tree-based Tucker rank:

$$\text{rank}_T(v) = (\text{rank}_\alpha(v); \alpha \in T) \quad \text{with } T \text{ a dimension tree}$$



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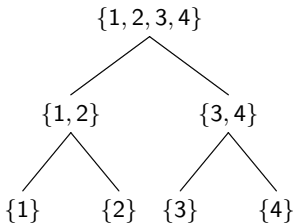
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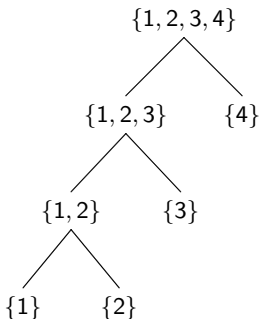
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- TT-rank:

$$\text{rank}_{TT}(v) = (\text{rank}_{\{1\}}(v), \text{rank}_{\{1,2\}}(v) \dots, \text{rank}_{\{1,\dots,d-1\}}(v))$$



$$\text{rank}_{TT}(v) \leq r = (r_1, \dots, r_{d-1}) \iff v = \sum_{i_1=1}^{r_1} \dots \sum_{i_{d-1}=1}^{r_{d-1}} v_{1,i_1}^1 \otimes v_{i_1,i_2}^2 \otimes \dots \otimes v_{i_{d-1},1}^d$$

- Different notions of rank yield different low-rank tensor subsets: Canonical, Tucker, Tree-based Tucker (HT, TT), ...

$$\mathcal{M}_{\leq r} = \{v \in V : \text{rank}(v) \leq r\}$$

- $\mathcal{M}_{\leq r}$ has a small dimension $n(r, d)$ (i.e. can be parameterized with a small number n of parameters), typically

$$n(r, d) = O(dr^5)$$

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Approximation in low-rank tensor subsets

- Good approximation properties for a large set of functions $C(V)$ of interest

$$\inf_{v \in \mathcal{M}} \|u - v\| \leq \epsilon(n) \quad \forall u \in C(V)$$

with rapidly decaying $\epsilon(n)$.

- Good approximation for smooth functions

Example (Sobolev regularity: approximation in canonical format)

$$\inf_{v \in \mathcal{R}_r} \|u - v\|_{L^2} \lesssim r^{-sd/(d-1)} \quad \forall u \in B_{mix}^s \subset L^2(\pi_d)$$

$$\text{with } B_{mix}^s = \left\{ u \in L^2(\pi_d); \|u\|_{H_{mix}^s} \leq 1 \right\} \subset H_{mix}^s(\pi_d)$$

That means that for any $u \in B_{mix}^s$ and for $\epsilon > 0$, it could be possible to find an approximation $v(x_1, \dots, x_d) = \sum_{i=1}^r \phi_i^1(x_1) \dots \phi_i^d(x_d)$ such that

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- But low-rank approximations are expected to **exploit additional features**.

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Best approximation in low-rank tensor subsets

- Best approximation problems in tree-based low-rank subsets $\mathcal{M}_{\leq r}$ are well-posed (provided some conditions on tensor norms).
- Best approximation problems related to singular value decompositions and their generalizations.
- For $d > 2$, no (guaranteed) algorithm for obtaining best approximations but for some tensor subsets (and particular norms), algorithms for obtaining quasi-best approximations

$$v_\gamma \in \mathcal{M} \quad \text{such that} \quad \|u - v_\gamma\| \leq (1 + \gamma(d)) \inf_{v \in \mathcal{M}} \|u - v\|$$

$$1 + \gamma(d) = \begin{cases} \sqrt{d} & \text{for Tucker tensors} \\ \sqrt{2d-2} & \text{for tree-based Tucker tensors} \end{cases}$$

(for Hilbert spaces equipped with the canonical norm)

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(for Hilbert spaces equipped with the canonical norm)

- Subsets of tensors with fixed tree-based rank have a manifold structure :

$$\mathcal{M}_{\leq r} = \bigcup_{s \leq r} \mathcal{M}_{=s}$$

$$\mathcal{M}_{=s} = \{v \in V : \text{rank}(v) = s\} = \left\{ v = F_{\mathcal{M}}(p) ; p = (p_1, \dots, p_L) \in \mathcal{P}^1 \times \dots \times \mathcal{P}^L \right\}$$

where $F_{\mathcal{M}}$ is a multilinear map and the \mathcal{P}^l are low-dimensional vector spaces (or manifolds).

- Interesting consequences:
 - Optimization algorithms on manifolds
 - Dynamical systems on low-rank manifolds



Falco, Hackbusch and Nouy.

Geometric structures in tensor representations. MIS Preprint.

Outline

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- 7 Higher-order low-rank methods for high-dimensional parametric and stochastic equations**

- Computation of an **output quantity of interest**

$$s(\xi) = \ell(u(\xi); \xi), \quad \xi \sim \mu,$$

$$s \in L^2_\mu(\mathbb{R}^d)$$

Sample-based low-rank tensor approximation

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- Best L^2 approximation in a low-rank subset \mathcal{M} (**not computable**)

$$\min_{v \in \mathcal{M}} \|s - v\|^2 = \min_{v \in \mathcal{M}} \mathbb{E}_\mu((s(\xi) - v(\xi))^2)$$

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- Suppose we have **evaluations $\{s(\xi^k)\}_{k=1}^K$** of s at **sample points $\{\xi^k\}_{k=1}^K$** (Simulations of the full order model or of a reduced order model).

Sample-based low-rank tensor approximation

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$$s \in L^2_\mu(\mathbb{R}^d)$$

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- Suppose we have **evaluations** $\{s(\xi^k)\}_{k=1}^K$ of s at **sample points** $\{\xi^k\}_{k=1}^K$ (Simulations of the full order model or of a reduced order model).
- Low rank approximation using **least-square minimization**:

$$\min_{v \in \mathcal{M}} \|s - v\|_K^2$$

$$\text{with } \|s - v\|_K^2 = \frac{1}{K} \sum_{k=1}^K (s(\xi^k) - v(\xi^k))^2 \approx \mathbb{E}_\mu((s(\xi) - v(\xi))^2)$$

- Regularization could be required

$$\min_{v \in \mathcal{M}} \|s - v\|_K^2 + \text{"regularization"}$$

Sample-based low-rank tensor approximation

- Regularization could be required

$$\min_{v \in \mathcal{M}} \|s - v\|_K^2 + \text{"regularization"}$$

- For a given tensor format

$$\mathcal{M} = \{v = F_{\mathcal{M}}(p_1, \dots, p_r); p_k \in \mathbb{R}^{m_k}, 1 \leq k \leq r\}$$

solve

$$\min_{p_1, \dots, p_r} \|s - F_{\mathcal{M}}(p_1, \dots, p_r)\|_K^2 + \sum_k \lambda_k \|p_k\|_s$$

that corresponds to a minimization in a subset of \mathcal{M} :

$$\mathcal{M}_{\gamma} = \{v = F_{\mathcal{M}}(p_1, \dots, p_r); p_k \in \mathbb{R}^{m_k}, \|p_k\|_s \leq \gamma_k, 1 \leq k \leq r\}$$

Sample-based low-rank tensor approximation

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- Sparsity-inducing regularization with $0 \leq s \leq 1$.

Now, entering the model...

Classical iterative methods with low-rank truncations

- Equation in tensor format

$$Bu = F, \quad u \in \mathcal{V} \otimes \mathcal{S}_1 \otimes \dots \otimes \mathcal{S}_d$$


- Iterative solver

$$u^{(k)} = T(u^{(k-1)}) \quad (T: \text{iteration map})$$

- Approximate iterations using low-rank truncations:

$$u^{(k)} \in \mathcal{M}_{r(\epsilon)} \quad \text{such that} \quad \|u^{(k)} - T(u^{(k-1)})\| \leq \epsilon$$

- For the canonical norm $\|\cdot\|$, truncation based on higher-order SVD
- Computational requirements: low-rank algebra and efficient truncation algorithms
- Analysis : perturbation of iterative algorithms.

(see  [Khoromskij & Schwab 2011])

- Residual-based error

$$\mathcal{E}(u, w) = \|Bw - F\|_C = \|w - u\|_{B^*CB}$$

with a certain residual norm $\|\cdot\|_C^2 = \langle C\cdot, \cdot \rangle$.

- Best approximation in $\mathcal{M}_{\leq r}$

$$\mathcal{E}(u, u_m) = \min_{w \in \mathcal{M}_{\leq r}} \mathcal{E}(u, w)$$

Approximation of higher-order tensors in canonical format

- Optimization in canonical format is ill-posed

$$\inf_{v \in \mathcal{R}_r} \mathcal{E}(u, v)$$

- A quasi-optimal approximation $u_r \in \mathcal{R}_r$ can be obtained (but usually numerically unstable)

$$\mathcal{E}(u, u_r) \leq (1 + \epsilon) \inf_{v \in \mathcal{R}_r} \mathcal{E}(u, v)$$

- No notion of decomposition

$$u_r = \sum_{i=1}^r u_i^{(1,r)} \otimes \dots \otimes u_i^{(d,r)}$$

Proper Generalized Decomposition in canonical format: greedy approximation

- Suboptimal construction of canonical representation using greedy algorithms.
- Starting from $u_0 = 0$, then

$$u_m = u_{m-1} + w_m$$

with $w_m = w_m^1 \otimes \dots \otimes w_m^d$ defined by


$$\mathcal{E}(u, u_{m-1} + w) = \min_{w \in \mathcal{R}_1} \mathcal{E}(u, u_{m-1} + w)$$

- Notion of decomposition

$$u_m = \sum_{i=1}^m w_i^1 \otimes \dots \otimes w_i^d$$

- Possible optimization of functions after each correction for improving convergence (but we loose the notion of decomposition).

Proper Generalized Decomposition : greedy approximation

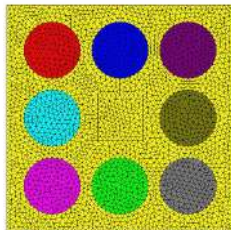
- Possible corrections w_m in other low-rank subsets.
- Convergence results available  [Cances & al 2011, Falco & N. 2012] (not really specific to tensor setting) but no a priori estimates.
- Convergence may be slow compared to $\inf_{w \in \mathcal{R}_r} \mathcal{E}(u, w)$
- The construction does not really exploit the tensor structure.

A simple illustration on a diffusion equation

$$\begin{cases} -\nabla \cdot (\kappa \nabla u) = I_D(x) & \text{on } \Omega = (0, 1) \times (0, 1) \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

$$\kappa(x, \xi) = \begin{cases} 1 & \text{if } x \in \Omega_0 \\ 1 + 0.1\xi_i & \text{if } x \in \Omega_i, i = 1 \dots 8 \end{cases}$$

with $\xi_i \in U(-1, 1)$



Approximation spaces

$$u \in \mathcal{V} \otimes \mathcal{S}, \quad \mathcal{S} = \mathbb{P}_{10}(-1, 1) \otimes \dots \otimes \mathbb{P}_{10}(-1, 1)$$

Underlying approximation space with dimension 5.10^{11}

Residual-based error

$$\mathcal{E}(u, v)^2 = \|v - u\|_B^2 = \mathcal{J}(v) - \mathcal{J}(u), \quad \mathcal{J}(v) = \int_{\Omega} \kappa \nabla v \cdot \nabla v - 2 \int_{\Omega} I_D v$$

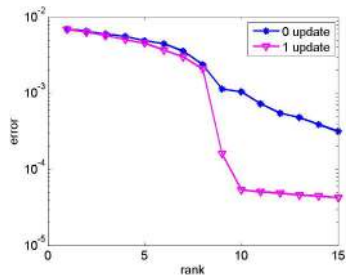
Progressive PGD

Progressive Galerkin PGD

$$u \approx u_m = \sum_{k=1}^m w_k, \quad w_k = v_k \otimes \phi_k^1 \otimes \dots \otimes \phi_k^s \in \mathcal{R}_1$$

$$\min_{w_m \in \mathcal{R}_1} \|u - u_{m-1} - w_m\|_B^2 \quad + \quad \text{updates of functions } \{\phi_k^1, \dots, \phi_k^s\}_{k=1}^m$$

Convergence (in L^2 norm)



Spatial modes w_k

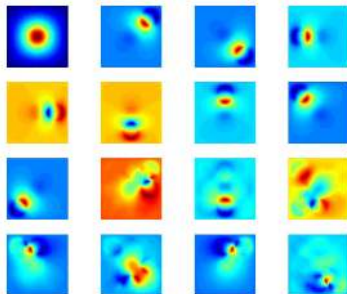
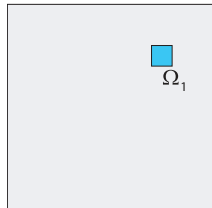


Illustration : stationary advection-diffusion-reaction equation

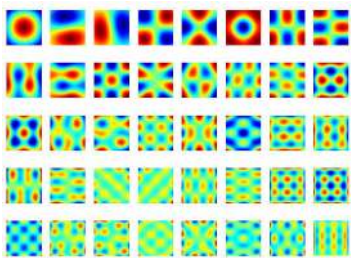
$$-\nabla \cdot (\kappa \nabla u) + c \cdot \nabla u + \gamma u = \delta l_{\Omega_1}(x) \quad \text{on } \Omega$$



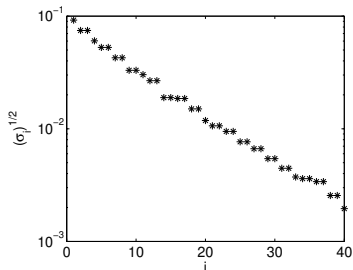
Random field

$$\kappa(x, \xi) = \mu_\kappa + \sum_{i=1}^{40} \sqrt{\sigma_i} \kappa_i(x) \xi_i, \quad \xi_i \in U(-1, 1)$$

Spatial modes $\kappa_i(x)$



Amplitudes σ_i



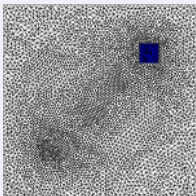
Stochastic approximation

$$\xi = (\xi_1, \dots, \xi_{40}), \quad \Xi = (-1, 1)^{40} = \Xi_1 \times \dots \times \Xi_{40}$$

$$\mathcal{S} = \mathbb{P}_4(\Xi_1) \otimes \dots \otimes \mathbb{P}_4(\Xi_{40})$$

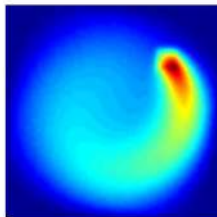
$$\dim(\mathcal{S}) = 5^{40} \approx 10^{28}$$

Finite element mesh



$$\dim(\mathcal{V}_N) = 4435$$

Solution $u(\cdot, \mu_\xi)$ for mean parameters



A basic hierarchical format

Deterministic/stochastic separation

$$u(\boldsymbol{\xi}) \approx u_m(\boldsymbol{\xi}) = \sum_{i=1}^m v_i s_i(\boldsymbol{\xi})$$

$$\hookrightarrow \mathcal{V}_m = \text{span}\{v_i\}_{i=1}^m$$

low-rank approximation of parametric functions

$$\mathbf{s}(\boldsymbol{\xi}) := (s_i)_{i=1}^m \approx \mathbf{s}_Z(\boldsymbol{\xi}) = \sum_{k=1}^Z \phi_k^0 \prod_{j=1}^d \phi_k^j(\xi_j)$$

$$\hookrightarrow \mathcal{S}_Z = \text{span}\{\prod_{j=1}^d \phi_k^j(\xi_j)\}_{k=1}^Z$$

For a precision $\|u - u_{M,Z}\|_{L^2} \leq 10^{-2}$

- $\dim(\mathcal{V}_m) \approx 15 \ll 4435 = \dim(\mathcal{V})$
- $\dim(\mathcal{S}_Z) \approx 10 \ll 10^{28} = \dim(\mathcal{S})$
- 15 classical deterministic problems in order to build $\mathcal{V}_M \subset \mathcal{V}_N$
- about 1 minute computation on a laptop with matlab

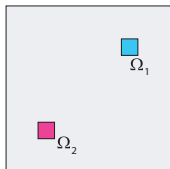
► Results

Convergence properties of quantities of interest

Probability of events

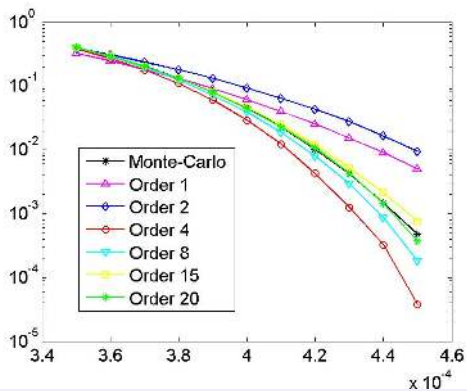
Quantity of interest

$$Q(\xi) = \int_{\Omega_2} u(x, \xi) dx$$



$$Q_M(\xi) = \int_{\Omega_2} u_M(x, \xi) dx$$

$P(Q > q), \quad q \in (3.5, 5.4)$



Convergence properties of quantities of interest

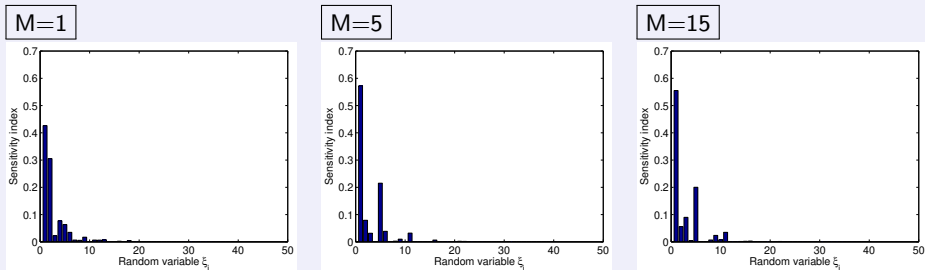
Sensitivity analysis

$$Q(\xi) \approx Q_M(\xi) \approx Q_{M,Z}(\xi) = \sum_{k=1}^Z q_k \Psi_k(\xi), \quad \Psi_k(\xi) = \prod_{i=1}^{40} \phi_k^i(\xi_i)$$

First order Sobol sensitivity index with respect to parameter ξ_i

$$S_i = \frac{\text{Var}(E(Q|\xi_i))}{\text{Var}(Q)} \quad E(Q|\xi_i) = \sum_{k=1}^Z \alpha_k^i \phi_k^i(\xi_i), \quad \alpha_k^i = q_k \prod_{\substack{j=1 \\ j \neq i}}^{40} E(\phi_k^j(\xi_j))$$

First order Sobol sensitivity indices S_i



Proper Generalized Decomposition for higher-order tensors: Tucker format

- Tucker tensors with bounded multilinear rank:

$$\begin{aligned}\mathcal{T}_r &= \{v : \text{rank}_\mu(v) \leq r_\mu, \forall \mu\} \\ &= \left\{ v \in \bigotimes_{\mu=1}^d U_\mu : \dim(U_\mu) \leq r_\mu, \forall \mu \right\}\end{aligned}$$

- Best approximation — a subspace point of view:

$$\min_{v \in \mathcal{T}_r} \mathcal{E}(u, v) = \min_{\dim(U_1)=r_1} \dots \min_{\dim(U_d)=r_d} \min_{v \in U_1 \otimes \dots \otimes U_d} \mathcal{E}(u, v)$$

This yields sequences of optimal but non necessarily nested subspaces $\{U_\mu^{r_\mu} : r_\mu \geq 1\}$.

- Greedy construction of subspaces with nestedness property

$$\mathcal{E}(u, u_m) = \min_{U_1^m \supset U_1^{m-1}} \dots \min_{U_d^m \supset U_d^{m-1}} \min_{v \in U_1^m \otimes \dots \otimes U_d^m} \mathcal{E}(u, v)$$

- Suboptimal greedy construction of subspaces with nestedness property (isotropic enrichment)  [Giraldi, Legrain and N. 2013]

$$\mathcal{E}(u, u_{m-1} + \otimes_{\mu=1}^d w_m^{(\mu)}) = \min_{w \in \mathcal{R}_1} \mathcal{E}(u, u_{m-1} + w), \quad U_\mu^m = U_\mu^{m-1} + \text{span}\{w_m^{(\mu)}\}$$

$$\mathcal{E}(u, u_m) \leq (1 + \epsilon) \min_{v \in U_1^m \otimes \dots \otimes U_d^m} \mathcal{E}(u, v)$$

- Greedy construction of subspaces with nestedness property (anisotropic enrichment)
At iteration m , select dimensions D_m for enrichment, let $U_\mu^m = U_\mu^{m-1}$ for $\mu \notin D_m$ and

$$\mathcal{E}(u, u_m) = \min_{\substack{U_\mu^m \supset U_\mu^{m-1} \\ \mu \in D_m}} \min_{v \in U_1^m \otimes \dots \otimes U_d^m} \mathcal{E}(u, v)$$

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Illustration: PDE with random coefficients

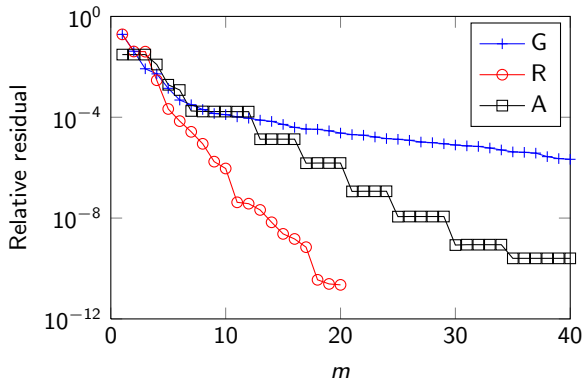
with Loic Giraldi

$$\begin{aligned} -\nabla \cdot (\nabla u) + \xi_2 u &= 1 \quad \text{on } D \setminus \omega \\ -\nabla \cdot ((1 + \xi_1)\nabla u) + \xi_2 u &= 1 \quad \text{on } \omega \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

$$\begin{aligned} \xi_1 &\sim U(0, 10), \quad \xi_2 \sim U(0, 1) \\ u &\in H_0^1(\Omega) \otimes L^2(\Xi_1) \otimes L^2(\Xi_2) \end{aligned}$$

Illustration: PDE with random coefficients

Error with respect to iteration for different tensor formats and algorithms



+ Greedy approximation in \mathcal{R}_r (rank-one updates)

o Suboptimal greedy construction of subspaces based on rank-one corrections (isotropic)

□ Suboptimal greedy construction of subspaces with anisotropic enrichment

Illustration: PDE with random coefficients

Ranks with respect to iteration m for anisotropic construction

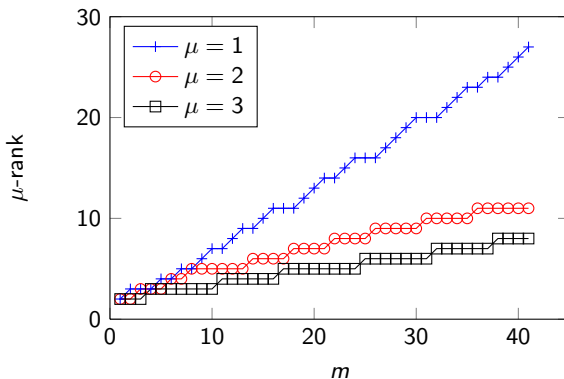
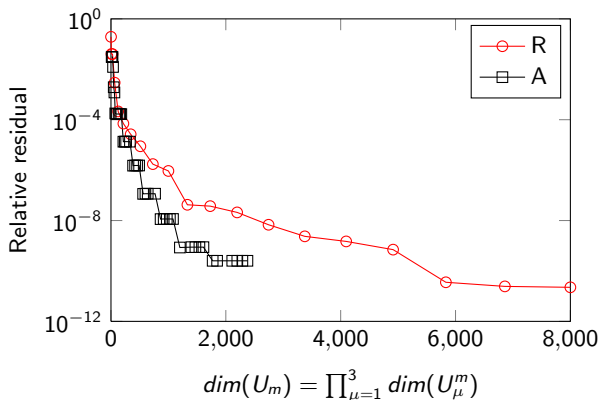


Illustration: PDE with random coefficients

Error with respect to the dimension of the reduced space U^m for greedy constructions of subspaces.



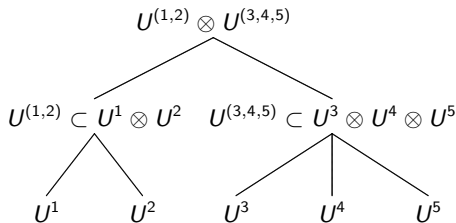
- Suboptimal greedy construction of subspaces based on rank-one corrections (isotropic)
- Suboptimal greedy construction of subspaces with anisotropic enrichment

Proper Generalized Decompositions for tree-based formats

- Tensors with bounded tree-based rank

$$\mathcal{H}_r^T = \{v : v \in U_\alpha \otimes U_{\alpha^c}, \dim(U_\alpha) \leq r_\alpha, \alpha \in T\}$$

s.t. the set of subspaces $\{U_\alpha\}_{\alpha \in T}$ has a hierarchical structure



- Best approximation problems - a subspace point of view

$$\min_{v \in \mathcal{H}_r^T} \|u - v\| = \min_{\substack{U_\mu \subset V_\mu \\ \dim(U_\mu) = r_\mu \\ \mu \in \{1, \dots, d\}}} \min_{\substack{U_\alpha \subset \bigotimes_{\beta \in S(\alpha)} U_\beta \\ \dim(U_\alpha) = r_\alpha \\ \alpha \in I(T)}} \min_{v \in \bigotimes_{\beta \in S(D)} U_\beta} \|u - v\|$$

define sequences of **optimal and non necessarily nested subspaces** $\{U_\alpha^{r_\alpha}; r_\alpha \geq 1\}$.

- Algorithms for the construction of suboptimal sequences of nested subspaces ... strategies of enrichment for non isotropic constructions ?

Challenging issues

- **Classify applications and dedicated reduced order methods**
 - Quantum physics : a long history for the construction of tensor formats
 - Machine learning and statistical learning: a huge literature on reduced order models for high dimensional functions.
- **A priori estimates**
- **Automatic selection of reduced order formats** (bases or frames for sparse approximation, tensor formats for low-rank approximation).
- **Well-conditioned formulations** for (quasi-)optimal model reduction
- **Samples-based constructions**: How to sample given an approximation format ? How many samples ?
- **Software engineering**. Minimize interactions with existing codes.
- **Goal-oriented model order reduction**: variable of interest $s = \ell(u)$, rare event computation, sensitivity analysis, optimization, inverse problems, ...

● LOW-RANK TENSOR METHODS



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● LOW-RANK FOR UQ AND PARAMETRIC MODELS



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