Model reduction methods for uncertainty quantification

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Outline

Uncertainty quantification

Uncertainty quantification has become an essential path in science and engineering

- Assess confidence in numerical predictions
- Comprehension and selection of models (exploration of model predictions over a range of uncertainty, sensitivity analysis)
- Robust optimization and design
- Validation of models from statistical data
- Data assimilation

Uncertainty quantification: stochastic models

Stochastic model

$$u : \theta \in \Theta \mapsto u(\theta) \in \mathcal{V} \quad \text{such that} \quad \mathcal{F}(u(\theta); a(\theta)) = 0$$

where uncertainties are represented by random parameters $a(\theta)$ defined on a probability space $(\Theta, \mathcal{B}, P)$.

- Forward problem:
  For a given probabilistic model for a, compute u or a quantity of interest $Q(u)$ (statistics, probability of events, sensitivity indices...)
- Inverse problem:
  For given observations, estimate a probabilistic model for a.

Uncertainty quantification using functional approaches

- Uncertainties modeled by “simple” random variables

$$\xi : \Theta \rightarrow \mathbb{R}^{N_\xi}, \quad \xi \sim \mu_\xi$$

- Functional representation of any $\sigma(\xi)$-measurable random variable

$$f(\theta) \equiv f(\xi(\theta))$$

- Functional expansions

$$f(\xi) \approx \sum_{j=1}^{N_\eta} \eta_j \psi_j(\xi) := f(\xi; \eta)$$

Stochastic (parametric) analyses

$$\text{Random parameters } a(\xi) = a(\xi;\eta), \quad \xi \sim \mu_\xi$$

- Forward problem : given μ_ξ and η, compute $\mathcal{O}(u)$ with

$$\mathcal{F}(u(\xi); a(\xi;\eta)) = 0$$

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- Forward problem : given μ_ξ and η, compute $\mathcal{O}(u)$ with

$$\mathcal{F}(u(\xi); a(\xi; \eta)) = 0$$

- Inverse problem: given $\mathcal{O}(u)$, determine $\eta \in \Xi_\eta \subset \mathbb{R}^{N_\eta}$ (or μ_η) with

$$\mathcal{F}(u(\xi, \eta); a(\xi; \eta)) = 0$$

Example: Diffusion in heterogeneous media

Stochastic PDE with a random diffusion matrix a:

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

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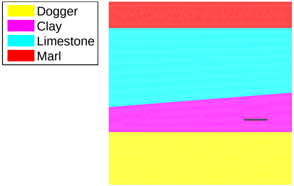
- Groundwater flow.
  Geological layers with uncertain properties:

$$a(x, \theta) = \sum_{i=1}^{4} \xi_i(\theta) I_{\Omega_i}(x)$$



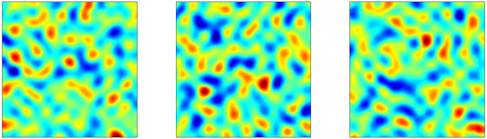
ξ_i's probability laws

Layer	Law
Dogger	$LU(5, 125)$
Clay	$LU(3.10^{-7}, 3.10^{-5})$
Limestone	$LU(1.2, 30)$
Marl	$LU(10^{-5}, 10^{-4})$

- Random media with spatially correlated random fields

$$a(x,\theta) = \underline{a}(x) + \sum_{i=1}^{m} \sqrt{\sigma_i}\varphi_i(x)\lambda_i(\xi(\theta)), \quad \xi = (\xi_1, \ldots, \xi_{N_\xi})$$

$$\lambda_i(\xi) = \sum_{\alpha} \eta_{i,\alpha}\psi_\alpha(\xi)$$



Uncertainty quantification using functional approaches

Ideal approach

Compute an accurate and explicit approximation of $u(\xi)$ (or $u(\xi, \eta)$) (metamodel, surrogate...) that allows fast evaluations of output quantities of interest, observables, or objective function.

Issue

Approximation of a high dimensional function

$$u(x), \; x \in \Xi \subset \mathbb{R}^d,$$

with $(\Xi, \mathcal{B}(\Xi), \mu)$ a measured space.

Outline

1. Uncertainty quantification
2. Model reduction methods for high dimensional problems
3. Sparse approximation
4. Tensor-structured problems and low-rank tensor approximation
5. Numerical methods for equations in tensor format
6. Low-rank approximation and subspace-based model reduction
7. Subspace-based model reduction for higher-order tensors

High dimensional problems

- Many problems in computational science requires the approximation of high dimensional functions:
$$u(x_1, \ldots, x_d)$$
- Classical discretization methods introduce high-dimensional parametrizations
$$u(x_1, \ldots, x_d) \approx \sum_{i_1=1}^{n_1} \ldots \sum_{i_d=1}^{n_d} a_{i_1 \ldots i_d} \varphi^1_{i_1}(x_1) \ldots \varphi^1_{i_d}(x_d)$$
$$a \in \mathbb{R}^{n_1 \times \ldots \times n_d}$$
- Model order reduction methods aim at replacing a complex model with a simplified one, living in a lower dimensional space (or manifold).

Model reduction methods

- 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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Model reduction methods

- 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
$$u(x_1^k, \ldots, x_d^k)$$
  - Equations (ODE, PDE, DAE)
  - Partial pointwise evaluations (e.g. for parametric/stochastic problems): equations for
$$u(\cdot, x_2^k, \ldots, x_d^k)$$

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Sparse approximation

- We want to approximate a function $u(x)$ in a certain vector space V equipped with a norm $\|\cdot\|$. Consider a set of functions $\{\psi_\alpha; \alpha \in \Lambda\}$ (called a dictionary) whose span is dense in V, so that

$$u(x) = \sum_{\alpha \in \Lambda} u_\alpha \psi_\alpha(x)$$

Typically, for multivariate functions

$$\psi_\alpha(x) = \psi^1_{\alpha_1}(x_1) \ldots \psi^d_{\alpha_d}(x_d), \quad \Lambda = \left\{\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d; \sum_{i=1}^d \alpha_i < \infty\right\}$$

- Sparse approximation methods rely on the fact that a good approximation (or even an exact decomposition) of the solution can be obtained by only considering a small subset of functions:

$$u(x) \approx u_n(x) = \sum_{\alpha \in \Lambda_n} u_\alpha \psi_\alpha(x), \quad \#\Lambda_n = n$$

Best n-term approximation

The best n-term approximation is the solution of

$$\inf_{u_n \in \mathcal{M}_n} \|u - u_n\| := \sigma_n(u)$$

where

$$\mathcal{M}_n = \left\{ v = \sum_{\alpha \in \Lambda_n} v_\alpha \psi_\alpha ; v_\alpha \in \mathbb{R}; \Lambda_n \subset \Lambda, \ \#\Lambda_n = n \right\}$$

- Selection of basis (or frame) suitable for a class of functions $\mathcal{K}$?

$$\sup_{u \in \mathcal{K}} \sigma_n(u) \leq c(n, \mathcal{K}) \underset{n \to \infty}{\longrightarrow} 0 \quad \text{with fast decay}$$

- Best n-term approximation is a combinatorial problem.
- Computation of the (quasi)-best n-term approximation through adaptive or non-adaptive algorithms ?

Sparse approximation: alternative strategies

- A priori definition of an index set $\widetilde{\Lambda}$, e.g. based on the properties of the class of functions we want to approximate (regularity, anisotropy...).
  - $\widetilde{\Lambda} = \{\alpha \in \mathbb{N}^d; \sum_{i=1}^d \alpha_i \leq p\}$
  - $\widetilde{\Lambda} = \{\alpha \in \mathbb{N}^d; \sum_{i=1}^d \gamma_i \alpha_i \leq p\}$ (anisotropic)
  - $\widetilde{\Lambda} = \{\alpha \in \mathbb{N}^d; \sum_{i=1}^d g(\alpha_i) \leq g(p)\}$ (smolyak)
  - ...

  A priori error estimation can be useful.
- Adaptive construction based on a posteriori error estimation, e.g. by greedy algorithms:

$$\Lambda_{n+1} = \Lambda_n \cup \{\alpha_{n+1}\}, \quad \text{with } \alpha_{n+1} \text{ in a candidate set.}$$

- Non-adaptive approximation by solving (approximately) the best n-term approximation problem.

$$\mathcal{M}_n = \{\sum_{\alpha\in\Lambda} v_\alpha \psi_\alpha ; \|\mathbf{v}\|_0 \leq n\} \xrightarrow{\text{convexification}} \mathcal{M}^\gamma = \{\sum_{\alpha\in\Lambda} v_\alpha \psi_\alpha ; \|\mathbf{v}\|_1 \leq \gamma\}$$

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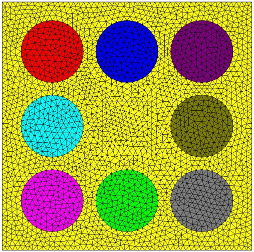
Illustration: diffusion problem with multiple inclusions

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



with

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

with $\xi_i \sim U(-1,1)$. $\Xi = (-1,1)^8$.

- Quantity of Interest:

$$I(\xi) = \int_D u(x,\xi)dx, \quad D = (0.4,0.6)\times(0.4,0.6)$$

- Polynomial approximation:

$$I(\xi) \approx \sum_{\alpha\in\Lambda} v_\alpha \psi_\alpha(\xi), \quad span\{\psi_\alpha : \alpha \in \Lambda\} = \mathbb{P}_4(\Xi), \quad dim(\mathbb{P}_4(\Xi)) = 1286$$

Coefficients $\{v_\alpha : \alpha \in \Lambda\}$ computed with least-squares with K samples.

$$\min_{\{I_\alpha\}} \sum_{k=1}^{K} (I(\xi^k) - \sum_{\alpha} v_\alpha \psi_\alpha(\xi^k))^2$$

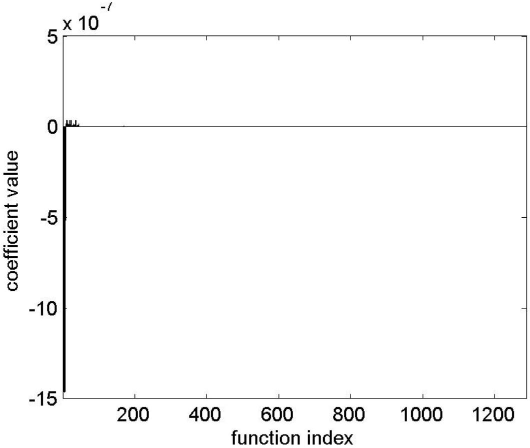


Figure : Values of the 1286 coefficients when using a large number of samples $K = 2000$

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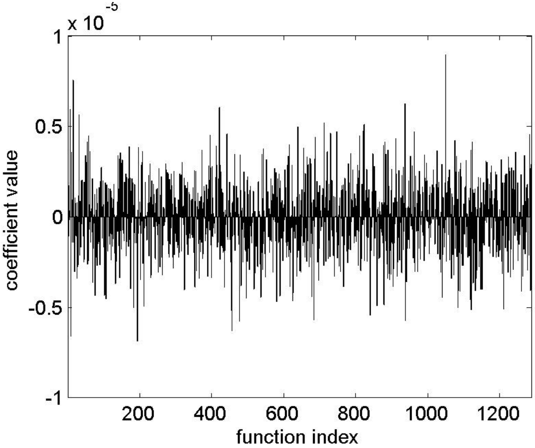
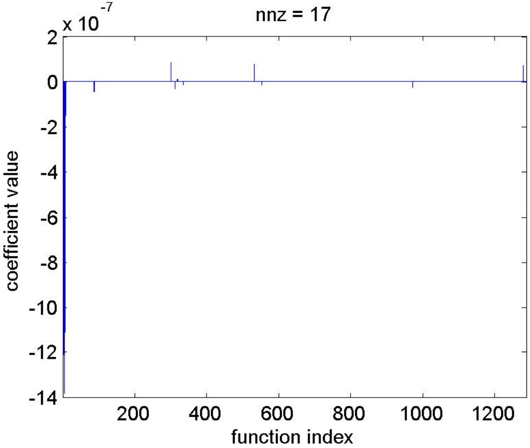


Figure : Values of the 1286 coefficients when using a small number of samples $Q = 50$

Least-squares with sparcity-inducing regularization (ℓ_1 regularization):

$$\min_{\{I_\alpha\}} \sum_{k=1}^{K} (I(\xi^k) - \sum_\alpha v_\alpha \psi_\alpha(\xi^k))^2 + \sum_\alpha |v_\alpha|$$



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Low rank tensor approximation :

What is a tensor ?

What is the rank of a tensor ?

Tensor spaces

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

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

or for multivariate functions

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

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

$$V_{\|\cdot\|} = \overline{V_1 \otimes_a \ldots \otimes_a V_d}^{\|\cdot\|}.$$

W. Hackbusch.
Tensor Spaces and Numerical Tensor Calculus,
Springer, 2012.

Examples of (Banach) tensor spaces

- Finite dimensional tensor spaces: For finite dimensional spaces,

$$V_{\|\cdot\|} = V = V_1 \otimes_a \ldots \otimes_a V_d$$

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

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

and identified with

$$a \in \mathbb{R}^{n_1 \times \ldots \times n_d} = \mathbb{R}^{n_1} \otimes \ldots \otimes \mathbb{R}^{n_d}$$

Examples of (Banach) tensor spaces

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

$$\|u\|_p = \left(\int_I \|u(y)\|^p_\mathcal{V}\mu(dy)\right)^{1/p} \qquad (1 \le p < \infty),$$

$$\text{or} \quad \|u\|_\infty = \operatorname*{ess\,sup}_{y\in I} \|u(y)\|_\mathcal{V} \qquad (p = \infty)$$

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

$$u(y) = \sum_{i=1}^m w_i \lambda_i(y), \quad y \in I.$$

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

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

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$$\overline{L^\infty_\mu(I) \otimes_a \mathcal{V}}^{\|\cdot\|_\infty} \subset L^\infty_\mu(I;\mathcal{V})$$

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Examples of (Banach) tensor spaces

- Lebesgue spaces $L^p_\mu(I)$ with product measures $\mu = \mu_1 \otimes \ldots \otimes \mu_d$ on $I = I_1 \times \ldots \times I_d$:

$$L^p_\mu(I_1 \times \ldots \times I_d) = \overline{L^p_{\mu_1}(I_1) \otimes_a \ldots \otimes_a L^p_{\mu_1}(I_d)}^{\|\cdot\|_p} \quad (1 \leq p < \infty)$$

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

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

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

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

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

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

Tensor-structured problems in Uncertainty Quantification

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

$$A_\xi(u(\xi)) = b_\xi, \quad u(\xi) \in \mathcal{V}$$

$$\xi \sim \mu, \quad supp(\mu) = \Xi$$

with parameter dependent operator A_ξ and right-hand side b_ξ.

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

- Functions of independent random variables:

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

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

$$u \in \mathcal{V} \otimes L^p_\mu(\Xi) = \mathcal{V} \otimes L^p_{\mu_1}(\Xi_1) \otimes \ldots \otimes L^p_{\mu_d}(\Xi_d)$$

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

$$u(\xi, \eta)$$

$$\xi \sim \mu, \quad supp(\mu) = \Xi, \quad \eta \in A$$

$$u \in \mathcal{V} \otimes L^p_\mu(\Xi) \otimes L^q_\nu(A)$$

- Stochastic calculus:

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

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

$$u(\cdot, t) \in H^1_{\mu_1}(\mathbb{R}) \otimes \ldots \otimes H^1_{\mu_n}(\mathbb{R})$$

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$$u \in \mathcal{V} \otimes L^p_\mu(\Xi) \otimes L^q_\nu(A)$$

- Stochastic calculus:

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

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

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

Other tensor structured problems in computational science

- Dynamical systems:

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

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

$$u \in L^p(I) \otimes \mathcal{V}$$

- Multidimensional PDEs

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

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

$$u \in H^1(\Omega_1) \otimes \ldots \otimes H^1(\Omega_d)$$

- 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

$$u \in \mathbb{R}^{2^d} \simeq \mathbb{R}^2 \otimes \ldots \otimes \mathbb{R}^2$$

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Low-rank approximation

- Approximation in a subset of tensors with bounded rank:

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

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

$$v \in V_1 \otimes V_2$$

$$rank(v) \leq r \iff v = \sum_{i=1}^{r} v_i^1 \otimes v_i^2 \quad \text{or} \quad v(x) = \sum_{i=1}^{r} v_i^1(x_1) v_i^2(x_2)$$

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

$$rank_\alpha(v) \leq r_\alpha \quad \Longleftrightarrow \quad v = \sum_{i=1}^{r_\alpha} v_i^\alpha \otimes v_i^{\alpha^c}, \quad v_i^\alpha \in V_\alpha, \quad v_i^{\alpha^c} \in V_{\alpha^c}$$

Example:

$u(x_1, \ldots, x_4) = f(x_1, x_2) g(x_3, x_4)$ is such that $rank_{(1,2)}(u) = rank_{(3,4)}(u) = 1$.

Higher-order low-rank formats

- Canonical rank:

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

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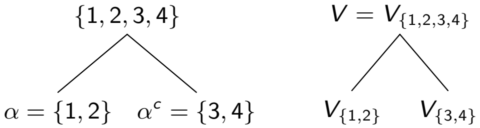

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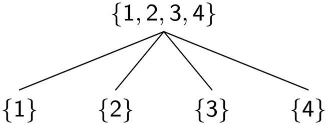
- Tucker rank:

$$rank_T(v) = (rank_1(v), \dots, rank_d(v))$$



$$rank_T(v) \leq r = (r_1, \dots, r_d) \iff v = \sum_{i_1=1}^{r_1} \dots \sum_{i_d=1}^{r_d} a_{i_1 \dots i_d} v^1_{i_1} \otimes \dots \otimes v^d_{i_d}$$

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$$rank_T(v) = (rank_\alpha(v); \alpha \in T) \quad \text{with } T \text{ a dimension tree}$$

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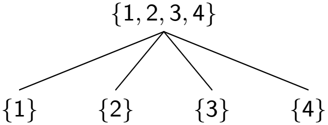

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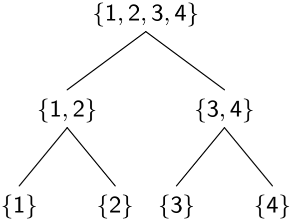
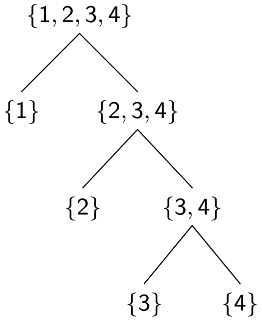


- TT-rank:

$$rank_{TT}(v) = (rank_1(v), \dots, rank_{d-1}(v))$$



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Low-rank tensor subsets

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

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

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

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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)

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

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

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

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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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Geometry of low-rank tensors

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

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

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

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

Equations in tensor format

Problem to solve

$$A(u) = b \quad \text{with} \quad u \in V = \bigotimes_{\mu=1}^{d} V_\mu$$

with

$$A = \sum_i \bigotimes_{\nu=1}^{d} A_i^\nu, \quad b = \sum_i \bigotimes_{\nu=1}^{d} b_i^\nu$$

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Example (Parametric PDE)

$$-a_1(\xi)\Delta u + a_2(\xi)u + a_3(\xi)c \cdot \nabla u = g(x)\phi(\xi), \quad x \in \Omega, \quad \xi \in \Xi, \quad u = 0 \quad on \quad \partial\Omega$$

recasted under the form

$$Au = b, \quad u \in H_0^1(\Omega) \otimes L_\mu^2(\Xi)$$

with

$$A = -\Delta \otimes A_1 + I \otimes A_2 + (c \cdot \nabla) \otimes A_3, \quad A_i : \lambda(\xi) \mapsto a_i(\xi)\lambda(\xi)$$

$$b = g \otimes \phi$$

Iterative solvers and low-rank tensor approximations

Given a low-rank format $\mathcal{M}$, replace an iterative solver

$$\{u_n\}_n \subset V \quad \text{s.t.} \quad u_n = B_n(u_{n-1})$$

with

$$\{u_n\}_n \subset \mathcal{M} \quad \text{s.t.} \quad u_n = T^{\epsilon}_{\mathcal{M}} B_n(u_{n-1})$$

where $T^{\epsilon}_{\mathcal{M}}$ is a "truncation operator" such that

$$\|T^{\epsilon}_{\mathcal{M}}(v) - v\| \leq \epsilon \|v\|$$

- When $\|\cdot\|$ is a canonical inner product norm, efficient algorihms based on SVD and controlled quasi-best approximations.
- Requires robustness of iterative solvers with respect to perturbations.
- Requires good preconditioners in tensor formats

Direct low-rank approximation

Given a low-rank tensor subset $\mathcal{M}$, replace

$$\inf_{v \in \mathcal{M}} \|u - v\|$$

by the optimization of a criterium

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

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- Natural minimization problems:

$$u = \arg\min_{v \in V} \mathcal{J}(v), \quad \mathcal{E}(u, v) = \mathcal{J}(v) - \mathcal{J}(u)$$

- Residual norms:

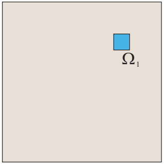
$$Au = b, \quad \mathcal{E}(u, v) = \|b - Av\|_*$$

- Sample-based semi-norms for stochastic/parametric problems:

$$\mathcal{E}(u, v) = \|u - v\|_K^2 + \text{“Regularization”} \quad \text{with} \quad \|u - v\|_K^2 = \sum_{k=1}^{Q} \|u(\xi^k) - v(\xi^k)\|^2$$

Illustration: advection-diffusion-reaction equation

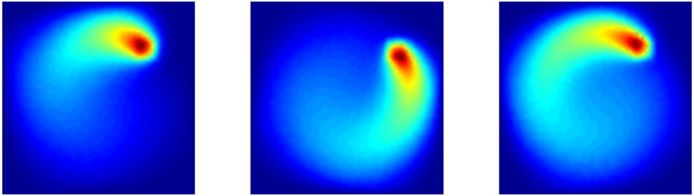
$$-a_1 \Delta u + a_2 u + a_3 c \cdot \nabla u = I_{\Omega_1} \quad on \quad \Omega$$
$$u = 0 \quad on \quad \partial\Omega$$



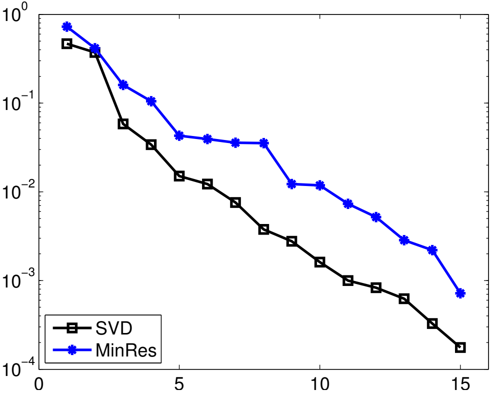
Uncertain parameters

$$a_1 = \mu_1(1 + 0.2\xi_1), \quad a_2 = \mu_2(1 + 0.2\xi_2), \quad a_3 = \xi_3$$
$$\xi_i \in U(-1, 1),\ \Xi = (-1, 1)^3$$

Samples of the solution $u(x, \boldsymbol{\xi})$



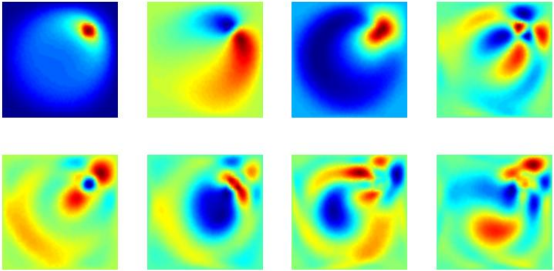
Convergence of best rank-m approximations in $L^2_\mu(\Xi;\mathcal{V})$-norm $\|\cdot\|$



$$u_m(x,\xi) = \sum_{i=1}^{m} w_i(x)\lambda_i(\xi)$$

- SVD: $u_m \in \arg\min_{v\in\mathcal{R}_m} \|u - v\|$
- MinRes: $u_m \in \arg\min_{v\in\mathcal{R}_m} \|Au - Av\|_*$ (canonical norm of the algebraic residual)

8 first spatial modes v_i of the SVD $u_m = \sum_{i=1}^{m} v_i \otimes \phi_i$



Direct approximation

If

$$\alpha\|u-v\| \leq \mathcal{E}(u,v) \leq \beta\|u-v\|$$

then

$$\tilde{u} = \arg\min_{v\in\mathcal{M}} \mathcal{E}(u,v)$$

is such that

$$\|u-\tilde{u}\| \leq \frac{\beta}{\alpha}\min_{v\in\mathcal{M}}\|u-v\|$$

Interest of working with well conditioned formulations,
i.e. such that $\beta/\alpha \approx 1$

- Construction of preconditioners in low-rank tensor formats (explicit preconditioning)

$$P = \sum_{i \in I} \alpha_i \bigotimes_{\mu=1}^{d} P^{\mu}_{i_\mu} \quad \text{(structured } \alpha\text{)}$$

[Giraldi, Nouy, Legrain 2013]

- Use non conventional minimal residual based formulations (implicit preconditioning)

$$A : V \to W', \quad \|Av - b\|_{W'} = \|v - u\|,$$

$$(1-\delta)\|u - v\| \leq \mathcal{E}(u, v) = \|\Lambda_\delta(Av - b)\|_{W'} \leq (1+\delta)\|u - v\|$$

[Cohen, Dahmen & Welper 2012]

[Billaud-Friess, Nouy & Zahm 2013]

Tensor approximation using statistical learning

- Computation of an output quantity of interest

$$f(\xi) = Q(u(\xi)), \quad \xi \sim \mu,$$

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Tensor approximation using statistical learning

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- Low rank approximation using least-square minimization:

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

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

where $\{f(\xi^k)\}_{k=1}^K$ are evaluations of f at sample points $\{\xi^k\}_{k=1}^K$ (Black-box deterministic computations).

Tensor approximation using statistical learning

- Regularization could be required

$$\min_{v \in \mathcal{M}} \|f - v\|_K^2 + \text{``regularization''}$$

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- 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

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

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

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

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

Outline

Low-rank approximation and subspace-based model reduction

- Rank-m tensor subset in $\mathcal{V} \otimes \mathcal{S}$

$$\mathcal{R}_m = \{v \in \mathcal{V} \otimes \mathcal{S} \; ; \; rank(v) \leq m\} = \left\{ v = \sum_{i=1}^{m} w_i \otimes \lambda_i ; w_i \in \mathcal{V}, \lambda_i \in \mathcal{S} \right\}$$

- Subspace point of view

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

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

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

This defines sequences of optimal subspaces $\mathcal{V}_m$ and $\mathcal{S}_m$.

Hilbert setting: induced norm and SVD

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

$$\langle w \otimes \lambda, w' \otimes \lambda' \rangle = \langle w, w' \rangle_{\mathcal{V}} \langle \lambda, \lambda' \rangle_{\mathcal{S}}.$$

- u is identified with an operator $u : w \in \mathcal{V} \to \langle u, w \rangle_{\mathcal{V}} \in \mathcal{S}$ which is compact and admits a singular value decomposition

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

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

$$u_m = \sum_{i=1}^{m} \sigma_i w_i \otimes \lambda_i$$

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

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

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

- Natural (induced) norm

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

- A rank-m approximation u_m is of the form

$$u_m(y) = \sum_{i=1}^{m} w_i \lambda_i(y)$$

- The best rank-m approximation u_m which solves

$$\min_{v \in \mathcal{R}_m} \|u - v\|^2$$

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

$$U\lambda = \int_\Xi u(y)\lambda(y)\mu(dy)$$

also known as Karhunen-Loeve decomposition (for y random variables) or Proper Orthogonal Decomposition (for y the time)

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

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

- The best rank-m approximation u_m which solves

$$\min_{v \in \mathcal{R}_m} \|u - v\|_K^2$$

corresponds to the truncated singular value decomposition of $U : \mathbb{R}^K \to \mathcal{V}$ defined by

$$U\alpha = K^{-1} \sum_{k=1}^{K} u(y^k)\alpha_k,$$

also known as Empirical Karhunen-Loeve decomposition (for y random variables) or Snapshots Proper Orthogonal Decomposition (for y the time)

Optimal low-rank approximation in the general case

In the general case (provided well-posedness of minimization problems), optimal spaces are still well defined by

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

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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

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

How to recover a notion of decomposition ?

Suboptimal constructions with nested subspaces and notion of decomposition

- Reduced Basis method (greedy algorithms) (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 $L^\infty \otimes L^\infty$)

Based on greedy constructions of the approximation or of subspaces.

Best rank-m approximation in $\mathcal{V} \otimes L^\infty_\mu(\Xi)$

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

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

- Optimal rank-m approximation is defined by

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

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

Best rank-m approximation in $\mathcal{V} \otimes L^\infty_\mu(\Xi)$

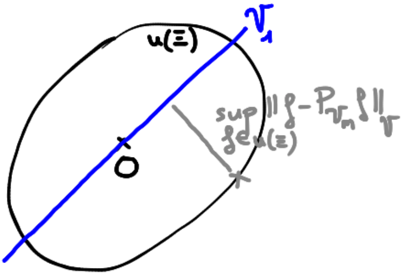
- Set of solutions

$$\mathcal{K} = \{u(y); y \in \Xi\} \subset \mathcal{V}$$

- Assuming $\mathcal{K}$ compact,

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

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



- In general, optimal spaces are such that

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

Greedy algorithm

Suboptimal construction of subspaces $\{\mathcal{V}_m\}_{m\geq 1}$ by imposing

- $\mathcal{V}_m \subset \mathcal{V}_{m+1}$
- $\mathcal{V}_m$ has a basis composed by pointwise evaluations of $u(\xi)$.

Greedy algorithm

Start with $u_0 = 0$ and for $m \geq 1$, do

- Compute $y_m \in \Xi$ such that

$$\|u(y_m) - u_{m-1}(y_m)\|_{\mathcal{V}} = \max_{y\in\Xi} \|u(y) - u_{m-1}(y)\|_{\mathcal{V}}$$

- Let $w_m = u(y_m)$ and $\mathcal{V}_m = span\{w_1, \dots, w_m\}$
- Let u_m such that

$$u_m(y) = P_{\mathcal{V}_m} u(y)$$

Reduced Basis method using greedy algorithm

- Parametric equation

$$A(u(y); y) = b(y)$$

- Minimization of a computable surrogate error

$$\mathcal{E}(u(y), v(y); y)$$

- Introduction of a discrete parameter set $\Xi_{train} \subset \Xi$

Greedy algorithm for Reduced Basis Method

Start with $u_0 = 0$ and for $m \geq 1$, do

- Compute $y_m \in \Xi_{train}$ such that

$$\mathcal{E}(u(y_m), u_{m-1}(y_m); y_m) = \max_{y \in \Xi_{train}} \mathcal{E}(u(y), u_{m-1}(y); y)$$

- Let $w_m = u(y_m)$ and $\mathcal{V}_m = span\{w_1, \ldots, w_m\}$
- Let u_m such that

$$\mathcal{E}(u(y), u_m(y); y) = \min_{v \in \mathcal{V}_m} \mathcal{E}(u(y), v; y)$$

Greedy algorithm and Reduced Basis method

Assuming

$$\alpha\|u-v\|_{\mathcal{V}} \leq \mathcal{E}(u,v;y) \leq \beta\|u-v\|_{\mathcal{V}},$$

and $\Xi = \Xi_{train}$, then

$$\|u(y_m)-u_{m-1}(y_m)\|_{\mathcal{V}} \geq \frac{\alpha}{\beta}\max_{y\in\Xi}\|u(y)-u_{m-1}(y)\|_{\mathcal{V}}$$

A quasi-optimality result [DeVore et al. 2012]

When $\mathcal{V}$ is a Hilbert space,

$$\|u-u_m\|_{\mathcal{V}} \leq \sqrt{2}\frac{\beta}{\alpha}\min_{1\leq i<m}(d_m(\mathcal{K};\mathcal{V}))^{\frac{m-i}{m}}$$

In particular

- $\|u-u_{2m}\|_{\mathcal{V}} \leq \sqrt{2}\frac{\beta}{\alpha}\sqrt{d_m(\mathcal{K};\mathcal{V})}$
- If $d_m(\mathcal{K};\mathcal{V}) \leq C_0 m^{-\delta}$, then $\|u-u_m\| \leq C_1 m^{-\delta}$ with $C_1 = 2^{5\alpha+1}\frac{\beta^2}{\alpha^2}C_0$
- If $d_m(\mathcal{K};\mathcal{V}) \leq C_0 e^{-c_0 m^\delta}$, then $\|u-u_m\| \leq \sqrt{2C_0}\frac{\beta}{\alpha}e^{-c_1 m^\delta}$ with $c_1 = 2^{-1-2\alpha}c_0$.

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

$$\|u - u_{m-1} - w_m \otimes \lambda_m\| = \min_{v \in \mathcal{R}_1} \|u - u_{m-1} - v\|$$

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

Proper Generalized Decomposition

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

$$\|u - u_{m-1} - w_m \otimes \lambda_m\| = \min_{v \in \mathcal{R}_1} \|u - u_{m-1} - v\|$$

$$u_m = \sum_{i=1}^{m} w_i \otimes \lambda_i \in \mathcal{V}_m \otimes \mathcal{S}_m, \quad \mathcal{V}_m = span\{w_i\}_{i=1}^m, \; \mathcal{S}_m = span\{\lambda_i\}_{i=1}^m$$

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

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

or partially greedy construction

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

- 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 Reduces Basis methods.

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- Suboptimal partial greedy construction of subspaces [Nouy 2007]

$$\|u - u_{m-1} - w_m \otimes \lambda_m\| = \min_{v \in \mathcal{R}_1} \|u - u_{m-1} - v\|$$

$$\|u - u_m\| = \min_{v \in \mathcal{V}_m \otimes \mathcal{S}} \|u - v\|, \quad \text{with} \quad \mathcal{V}_m = span\{w_i\}_{i=1}^m$$

$$u_m = \sum_{j=1}^{m} w_i \otimes \lambda_i^m$$

Greedy construction of a reduced basis $\{w_1, \dots, w_m, \dots\}$.

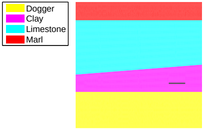
Example: stochastic Groundwater flow equation (MOMAS/Couplex)

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

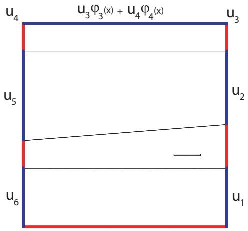


κ's probability laws

Layer	Law
Dogger	$LU(5, 125)$
Clay	$LU(3.10^{-7}, 3.10^{-5})$
Limestone	$LU(1.2, 30)$
Marl	$LU(10^{-5}, 10^{-4})$

10 basic uniform random variables ξ, $\Xi = (-1,1)^{10}$, uniform probability P_ξ

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	$U(285, 287)$

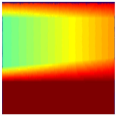
Progressive PGD

$$u_m(x,\xi) = \sum_{i=1}^{m} w_i^1(x) w_i^2(\xi)$$

Computing $(w_1^1(x), w_1^2(\xi))$ by alternated direction algorithm

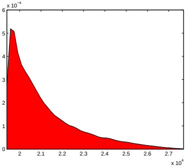
Initialize w^2 and alternate $w^1 = f_1^1(w^2)$ and $w^2 = f_1^2(w^1)$

$w^1 = f_1^1(w^2)$



$\downarrow$

$w^2 = f_1^2(w^1)$



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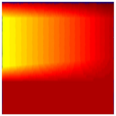

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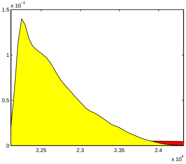

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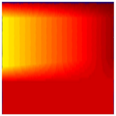

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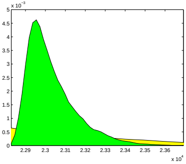

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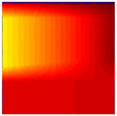

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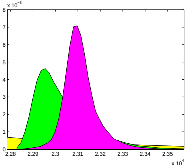

$$u_m(x,\xi) = \sum_{i=1}^{m} w_i^1(x) w_i^2(\xi)$$

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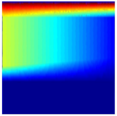

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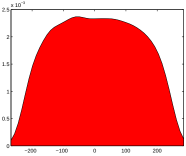

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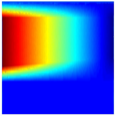

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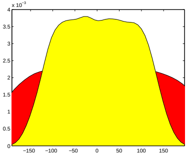

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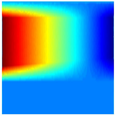

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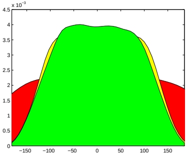

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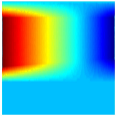

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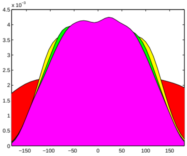

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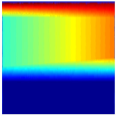
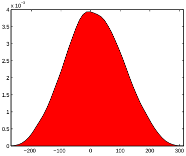


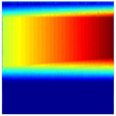
$\downarrow$

$w^2 = f_3^2(w^1)$



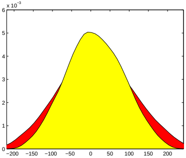
$\nearrow$

$w^1 = f_3^1(w^2)$



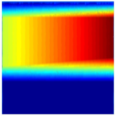
$\downarrow$

$w^2 = f_3^2(w^1)$



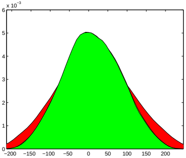
$\nearrow$

$w^1 = f_3^1(w^2)$



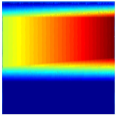
$\downarrow$

$w^2 = f_3^2(w^1)$



$\nearrow$

$w^1 = f_3^1(w^2)$



$\downarrow$

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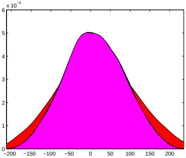
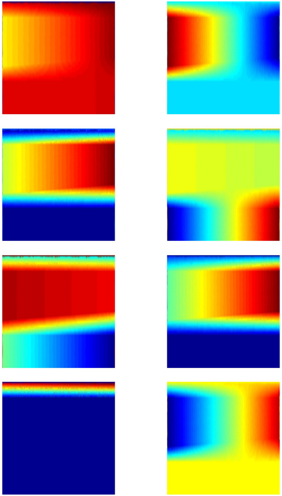
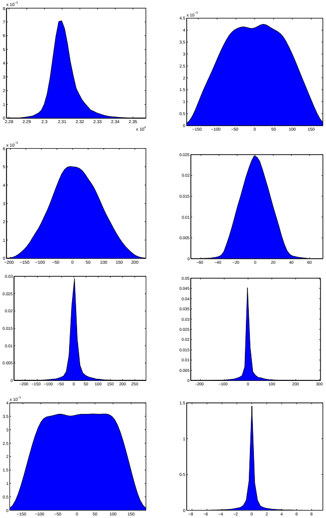


First modes of the progressive PGD

Spatial modes $\{w_1^1, \dots, w_8^1\}$

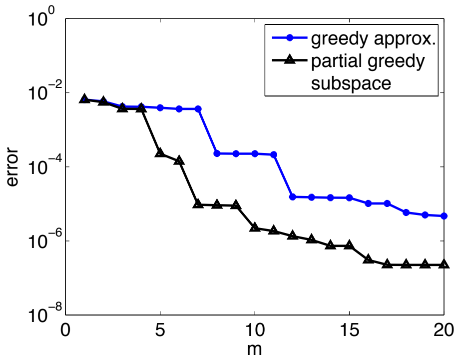


Stochastic modes $\{w_1^2, \dots, w_8^2\}$



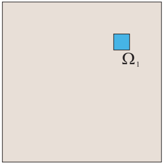
Convergence of the progressive PGD (L^2-norm)

$$\|u - u_m\|_{L^2(\Omega\times\Xi)}$$



Application to an advection-diffusion-reaction equation

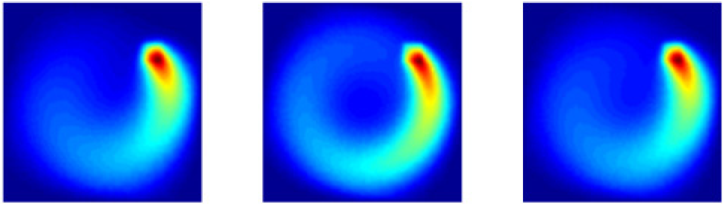
- $\partial_t u - a_1 \Delta u + a_2 c \cdot \nabla u + a_3 u = a_4 I_{\Omega_1}$ *on* $\Omega \times (0, T)$
- $u = 0$ *on* $\Omega \times \{0\}$
- $u = 0$ *on* $\partial\Omega \times (0, T)$



Uncertain parameters

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

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



Application to an advection-diffusion-reaction equation

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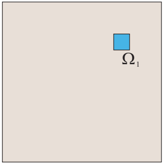


Uncertain parameters

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

Low-rank approximation of the solution

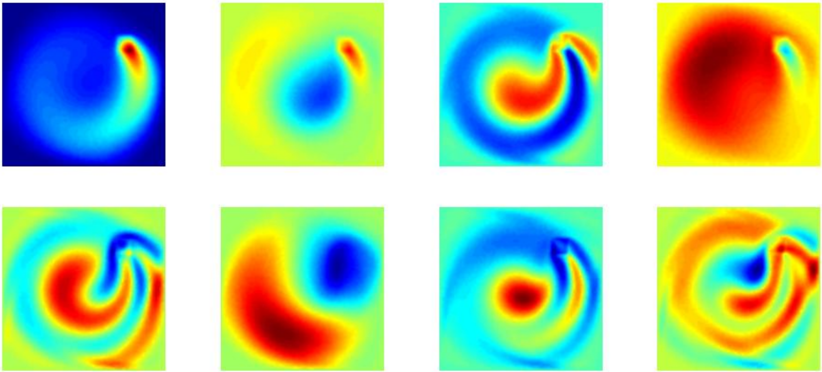
$$\boxed{u(x, t, \boldsymbol{\xi}) \approx \sum_{i=1}^{M} w_i(x, t)\lambda_i(\boldsymbol{\xi})}$$

$$w_i \in \mathcal{V} = L^2(0, T; H_0^1(\Omega)), \quad \lambda_i \in \mathcal{S} = L^2_{P_\xi}(\boldsymbol{\Xi})$$

Generalized Spectral Decomposition

Approximation of the ideal pseudo eigenspace through Arnoldi-type procedure

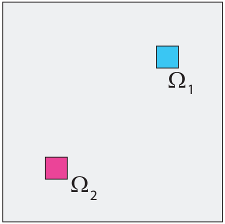
8 first modes of the decomposition $\{w_1(x,t) \ldots w_8(x,t)\}$



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

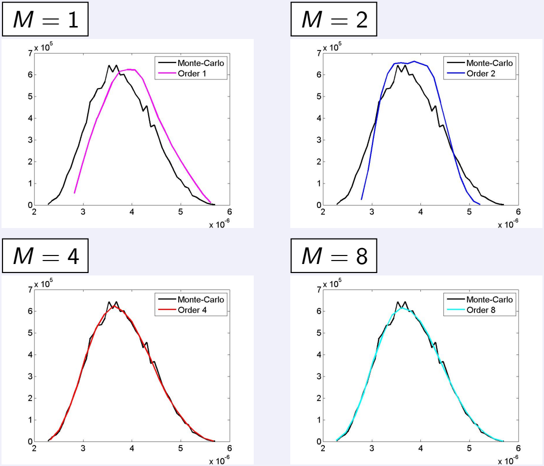
Quantity of interest

$$Q(\boldsymbol{\xi}) = \int_0^T \int_{\Omega_2} u(x, t, \boldsymbol{\xi})\, dxdt$$



$$Q_M(\boldsymbol{\xi}) = \int_0^T \int_{\Omega_2} u_M(x, t, \boldsymbol{\xi})\, dxdt$$

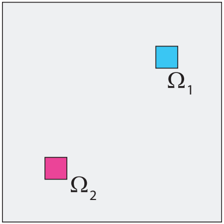
Probability density function of $Q_M(\boldsymbol{\xi})$



Convergence of quantities of interest
Quantiles

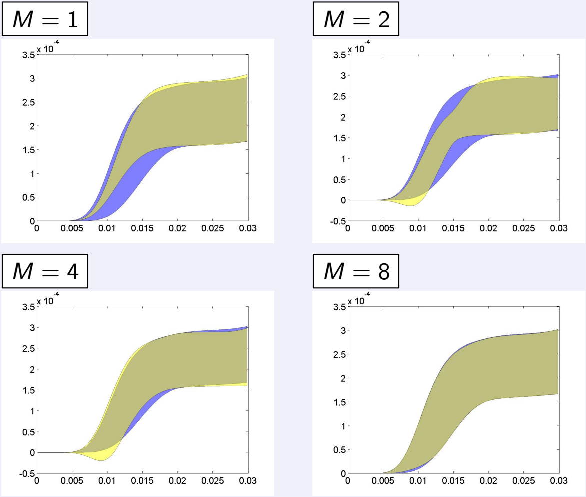
Quantity of interest

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

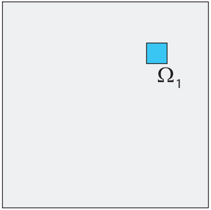


$$Q_M(t,\boldsymbol{\xi}) = \int_{\Omega_2} u_M(x,t,\boldsymbol{\xi})\,dx$$

99% Quantiles of $Q_M(t,\boldsymbol{\xi})$



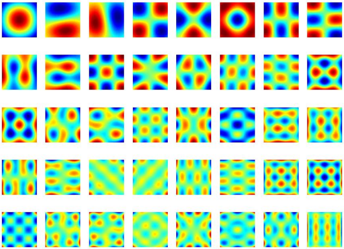
$$-\nabla \cdot (\kappa \nabla u) + c \cdot \nabla u + \gamma u = \delta I_{\Omega_1}(x) \quad on \quad \Omega$$



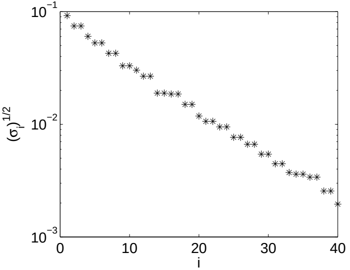
Random field

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

Spatial modes $\kappa_i(x)$



Amplitudes σ_i



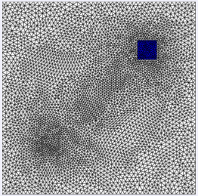
Stochastic approximation

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

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

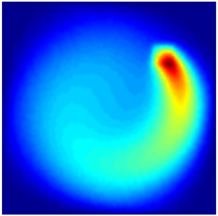
$$\boxed{dim(\mathcal{S}_P) = 5^{40} \approx 10^{28}}$$

Finite element mesh



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

Solution $u(\cdot, \boldsymbol{\mu}_{\boldsymbol{\xi}})$ for mean parameters



A basic hierarchical format

Deterministic/stochastic separation

$$u(\boldsymbol{\xi}) \approx u_M(\boldsymbol{\xi}) = \sum_{i=1}^{M} w_i \lambda_i(\boldsymbol{\xi})$$

$\hookrightarrow$ $\boxed{\mathcal{V}_M = span\{w_i\}_{i=1}^M}$

Random variables separation

$$\Lambda(\boldsymbol{\xi}) := (\lambda_i)_{i=1}^M \approx \Lambda_Z(\boldsymbol{\xi}) = \sum_{k=1}^{Z} \phi_k^0 \prod_{j=1}^{s} \phi_k^j(\xi_j)$$

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

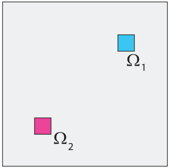
For a precision $\|u - u_{M,Z}\|_{L^2} \leqslant 10^{-2}$

- $\boxed{dim(\mathcal{V}_M) \approx 15} \ll 4435 = dim(\mathcal{V}_N)$
- $\boxed{dim(\mathcal{S}_Z) \approx 10} \ll 10^{28} = dim(\mathcal{S}_P)$
- 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

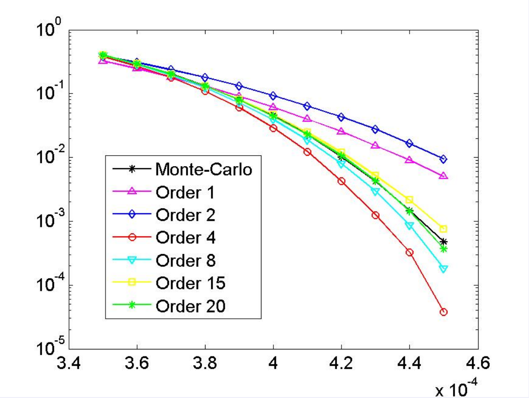
Quantity of interest

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



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

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



Convergence properties of quantities of interest

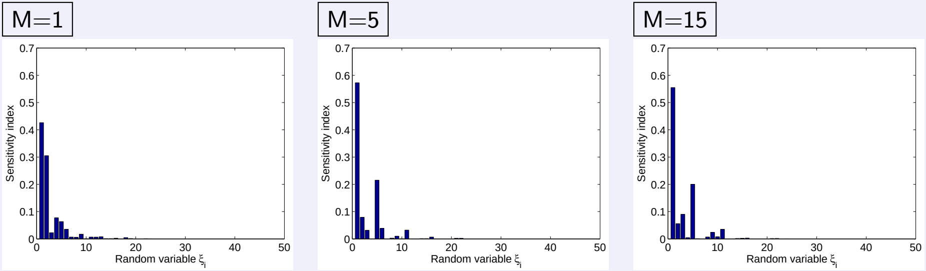
Sensitivity analysis

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

First order Sobol sensitivity index with respect to parameter ξ_i

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

First order Sobol sensivity indices S_i



Outline

- Tucker tensors with bounded multilinear rank:

$$\mathcal{T}_r = \{v : rank_\mu(v) \leq r_\mu, \forall \mu\} = \left\{ v \in \bigotimes_{\mu=1}^{d} U_\mu \; : \; dim(U_\mu) \leq r_\mu, \forall \mu \right\}$$

- 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 $\{U_\mu^{r_\mu} : r_\mu \geq 1\}$.

Proper Generalized Decomposition for higher-order tensors

- 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]

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

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

- 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

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

Proper Generalized Decomposition for higher-order tensors

- Greedy construction of subspaces with nestedness property

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

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Proper Generalized Decomposition for higher-order tensors

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

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

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

- 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

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

Simple Benchmark: Poisson equation

$$-\Delta u = 1 \quad \text{on} \quad \Omega = (0,1)^d$$

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

$$\mathcal{E}(v,u) = \|v-u\|^2_{H^1_0}$$

- Tensor-structured operator

$$\Delta = \partial_1^2 \otimes I \otimes \ldots \otimes I + \ldots + I \otimes \ldots \otimes I \otimes \partial_d^2$$

- Finite element space $V = V_1 \otimes \ldots \otimes V_d \subset H^1_0(\Omega)$.
- Galerkin approximation $u \in V$: tensor structured algebraic equation

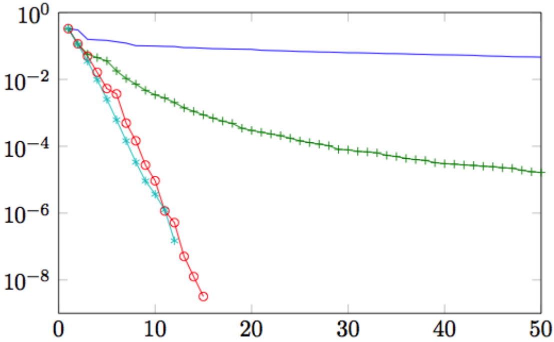
$$Au = b,$$

$$A = K \otimes M \otimes \ldots \otimes M + \ldots + M \otimes \ldots \otimes M \otimes K,$$

$$b = a \otimes \ldots \otimes a$$

Simple Benchmark: Poisson equation in dimension $d = 8$

Error with respect to the rank for different tensor formats and algorithms



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

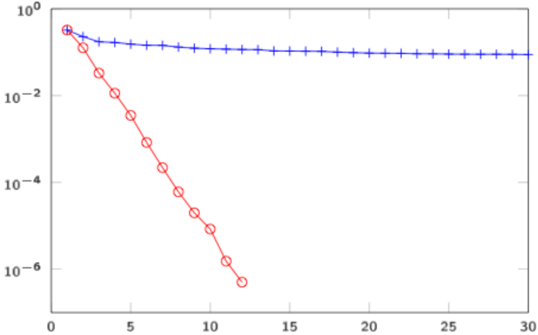
$+$ "Optimal approximation" $\mathcal{R}_r$

$\star$ Optimal approximation in $\mathcal{H}_r(V_1 \otimes \ldots \otimes V_d)$

$\circ$ Suboptimal greedy construction of subspaces U_μ^r (approximation in $\mathcal{H}_r(U_1^r \otimes \ldots \otimes U_d^r)$)

Simple Benchmark: Poisson equation in dimension $d = 27$

Error with respect to the rank for different tensor formats and algorithms



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

$\circ$ Suboptimal greedy construction of subspaces U_μ^r (approximation in $\mathcal{H}_r(U_1^r \otimes \ldots \otimes U_d^r)$)

Illustration: PDE with random coefficients

$$-\nabla \cdot (K \nabla u) + \xi_2 u = 1 \quad on \quad \Omega, \quad u = 0 \quad on \quad \partial\Omega$$

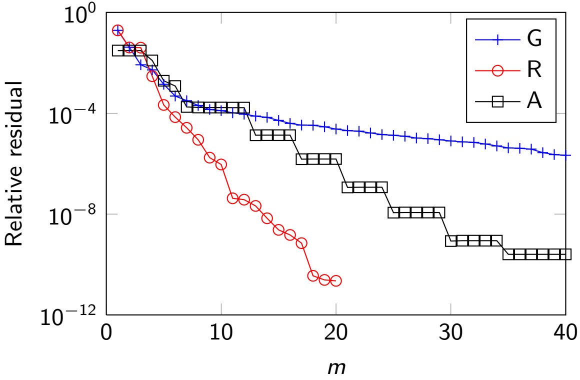
$$K = 1 + \xi_1 I_D(x)$$

$$\xi_1 \sim U(0, 10), \quad \xi_2 \sim U(0, 1)$$

$$u \in H_0^1(\Omega) \otimes L^2(\Xi_1) \otimes L^2(\Xi_2)$$

Illustration: PDE with random coefficients

Error with respect to iteration for different tensor formats and algorithms

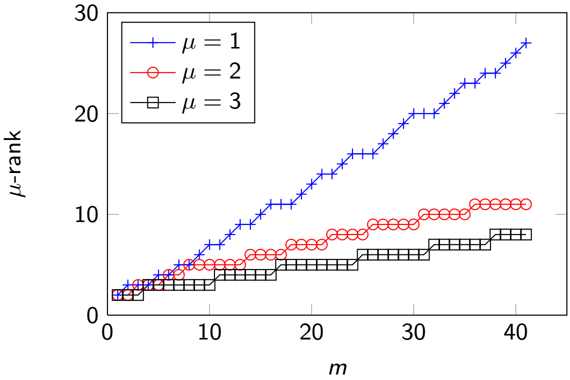


+ Greedy approximation in $\mathcal{R}_r$ (rank-one updates)

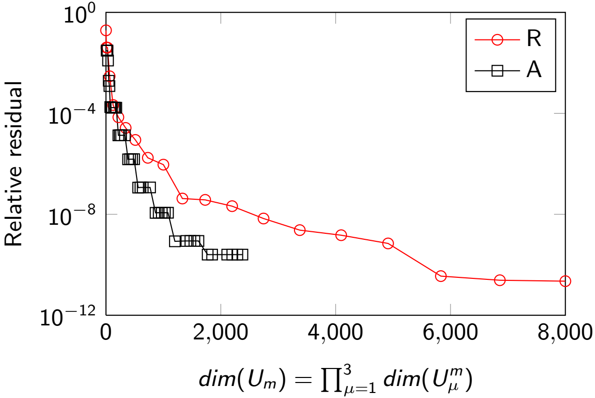
○ Suboptimal greedy construction of subspaces based on rank-one corrections (isotropic)

□ Suboptimal greedy construction of subspaces with anisotropic enrichment

Ranks with respect to iteration m for anisotropic construction



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)

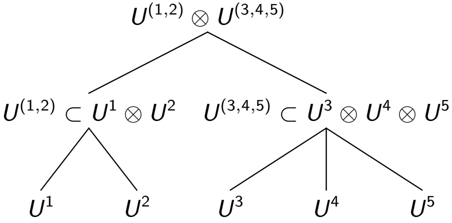
□ Suboptimal greedy construction of subspaces with anisotropic enrichment

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: quantity of interest $Q(u)$, rare event computation, sensitivity analysis, optimization, inverse problems, ...

References I

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