Uncertainty Quantification and Model Reduction

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Outline

Uncertainties

Many models contain uncertainties that may be

- aleatoric, random and not reducible,
- epistemic, due to lack of knowledge, reducible by adding information.

Probability theory as a mathematical theory for modeling

- aleatoric uncertainty: frequentist point of view,
- and also epistemic uncertainty: probability arises from information theory (Cox's theorem, maximum of entropy), Bayesian point of view

Uncertainty quantification

Uncertainty quantification has become an essential path in science and engineering.

- Predictive modelling and simulation under uncertainty
- Interplay between numerical analysis, scientific computing, probability and statistics

Objectives:

- Assess confidence in model predictions
- Comprehension and selection of models (exploration of model predictions over a range of uncertainty, sensitivity analysis)
- Robust optimization, control

Uncertainty quantification

Requires an accurate description of input uncertainties. Probabilistic model must be constructed objectively based on

- prior information,
- and/or available data.

As an example, consider a diffusion model

$$-\nabla \cdot (a \nabla u) = f$$

with uncertain diffusion coefficient a.

- Prior information and possible use of maximum of entropy principle:
  - positive definite matrix (second law of thermodynamics) with possible symmetries (isotropy, orthotropy...), bounds, ...
  - stationarity, correlation structure...
- If data available, statistical inference or bayesian update of prior models. Data usually given as indirect observations with uncertainties.

Uncertainty quantification

Stochastic model

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

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

- Forward problem: given μ, compute a variable of interest

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

  and quantities of interest (statistical moments, probability of events, sensitivity indices...).
- Inverse problem: given observations of $s(\xi)$, estimate μ.

Computational approaches for forward problems

Different computational approaches:

- Direct integration : compute statistics using integration, e.g. with Monte-Carlo methods, Quasi-Monte-Carlo methods or other quadrature methods...
- Moment methods: equations for statistical moments, e.g. using perturbation methods
- Probability distributions : equations for probability densities, e.g. Kolmogorov equations
- Direct approximation : compute an approximation of $u(\xi)$ and then evaluate (quickly) output variables of interest, observables, or objective function. Approximation known as reduced order model, metamodel, surrogate model...

Complexity issues for high-dimensional problems

Complexity issues for direct approximation

- Complex numerical models

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

$$\dim(V) \gg 1$$

  - Limit the number of sample evaluations
  - Remedy: projection-based model reduction, approximation of $u(\xi)$ in a low-dimensional subspace (or manifold) of V

- Approximation of multivariate functions

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

$$d \gg 1 \text{ (possibly } d = \infty)$$

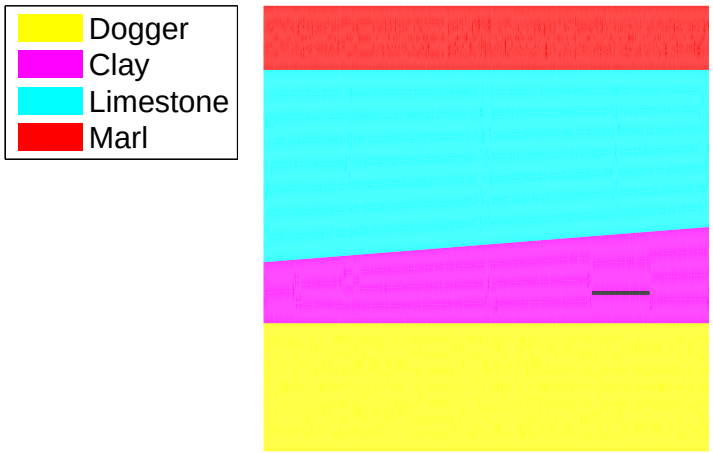
  - Classical approaches suffer from the curse of dimensionality
  - Remedy: adapted bases, structured approximations

Outline

An introductive example

Groundwater flow equation.

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



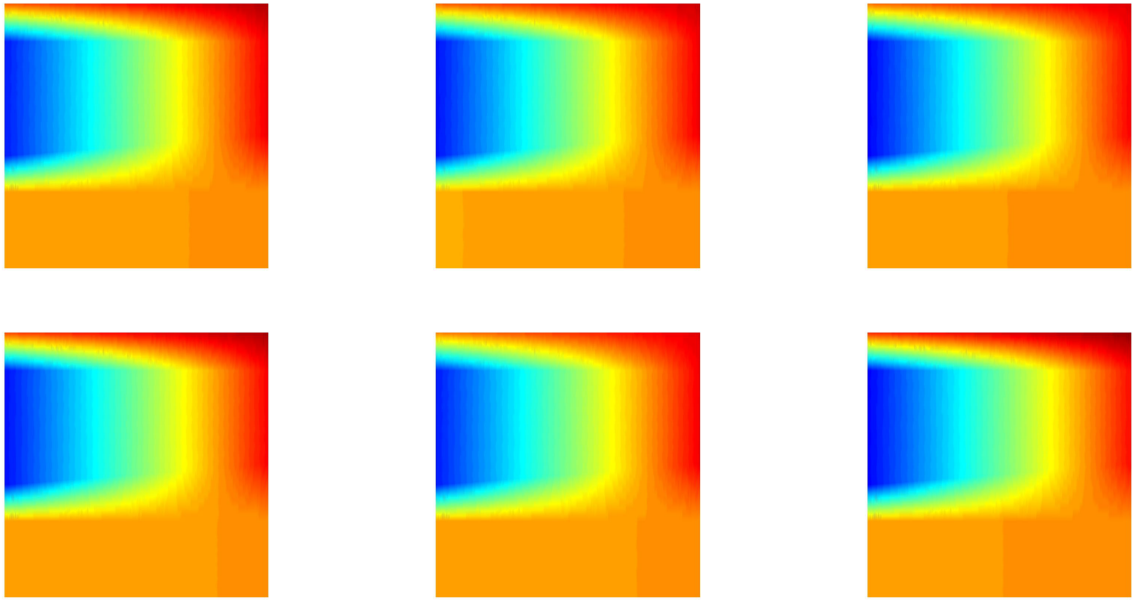
$$a(x, \xi) = \sum_{k=1}^{4} \xi_k I_{D_k}(x)$$

Layer	Random diffusion coefficient
D_1 : Dogger	$\xi_1 \sim LU(5, 125)$
D_2 : Clay	$\xi_2 \sim LU(3.10^{-7}, 3.10^{-5})$
D_3 : Limestone	$\xi_3 \sim LU(1.2, 30)$
D_4 : Marl	$\xi_4 \sim LU(10^{-5}, 10^{-4})$

Problem requiring fine discretization :

$$u(\xi) \in V, \quad \dim(V) \gg 1$$

- Samples $\{u(\xi^i)\}_{1\leq i\leq m}$ of the solution $u(\xi)$.



- Low-dimensionality of the set of solutions $u(\xi)$ that should be well approximated on low-dimensional subsets.
- Interpolation as a first idea

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

Worst case error

$$\epsilon_m^{(\infty)} = \sup_{\xi} \|u(\xi) - u_m(\xi)\|$$

m	1	3	6	10
$\epsilon_m^{(\infty)}/\epsilon_0^{(\infty)}$	2.10^{-2}	8.10^{-3}	4.10^{-4}	1.10^{-6}

Model order reduction for parametric problems

$$u : \Xi \to V \quad \text{such that} \quad A(u(\xi); \xi) = f(\xi), \quad \xi \in \Xi$$

- Linear methods: approximation in a low-dimensional subspace

$$V_m = span(v_1, \ldots, v_m) \subset V$$

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

- Nonlinear methods: approximation in a low-dimensional manifold

$$V_m \subset V$$

$$u_m(\xi) = R(s_1(\xi), \ldots, s_m(\xi)) \quad \text{with} \quad R : \mathbb{R}^m \to V_m \text{ (parametrization of } V_m)$$

How to quantify optimal reduction methods ?

- How to measure the quality of a space (or manifold) V_m ?

$$\text{for } \xi \in \Xi, \quad d(u(\xi), V_m) = \inf_{v \in V_m} \|u(\xi) - v\|$$

  - Worst case error ($L^\infty(\Xi)$)

$$\sup_{\xi \in \Xi} d(u(\xi), V_m)$$

  - Averaged error ($L^p_\mu(\Xi)$)

$$\left(\int_\Xi d(u(\xi), V_m)^p \mu(d\xi) \right)^{1/p}$$

  - ...

- The ideal performance of a reduction method can be quantified by measuring the "width" of the solution manifold

$$K = \{u(\xi) : \xi \in \Xi\} \subset V$$

Linear widths (resp. nonlinear widths) measure how well K can be approximated by a linear space (resp. manifold)

How to quantify optimal reduction methods ?

- Kolmogorov width (linear width for $L^\infty(\Xi)$-optimality)

$$d_m(K) = \inf_{\dim(V_m)=m} \sup_{\xi\in\Xi} d(u(\xi), V_m)$$

Provides a benchmark for optimal reduced basis methods : if $d_m(K) \leq \epsilon$, there exists a m-dimensional space such that

$$d(u(\xi), V_m) \leq \epsilon \quad \text{for all } \xi$$

- Linear width for $L^p_\mu(\Xi)$-optimality

$$\sigma_m^{(p)}(u) = \inf_{\dim(V_m)=m} \left(\int_\Xi d(u(\xi), V_m)^p \mu(d\xi) \right)^{1/p}$$

The case $p = 2$ corresponds to singular value decomposition (Karhunen-Loeve decomposition) of u.

- Non-linear width measures how well K can be approximated by a manifold. Devore-Howard-Michelli width defined by

$$\delta_m(K) = \inf_{R,C} \sup_{\xi\in\Xi} \|u(\xi) - R(C(u(\xi)))\|$$

where the infimum is taken over all continuous maps $C : K \to \mathbb{R}^m$ and $R : \mathbb{R}^m \to V$.

How to quantify optimal reduction methods ?

How fast m-widths go to zero with m ?

- Some general results in approximation theory (usually exploiting smoothness).
- Some finer results for particular cases.

Behaviour of m-widths

Consider the parametric model

$$-\nabla \cdot (a(x,\xi)\nabla u(\xi)) = f \quad \text{in } D \subset \mathbb{R}^d, \quad u(\xi) = 0 \quad \text{on } \partial D$$

$$0 < \alpha \leq a(x,\xi) \leq \beta < \infty$$

- A general result.

$$K \subset H_0^1(D) = V$$

If $f \in H^{s-1}(D)$ and $a(\cdot,\xi) \in C^s$, then $u(\xi) \in H^{s+1}$ and

$$d_m(K) \lesssim m^{-s/d}$$

Behaviour of m-widths

- Finer results taking into account the particular parametrization

$$a(x,\xi) = a_0(x) + \sum_{i=1}^{r} a_i(x)\xi_i, \quad \xi_i \in (-1,1)$$

  - $r < \infty$: Exponential convergence of $d_m(K)$. Deterioration of the rate with r.
  - $r = \infty$: If $(\|a_i\|_\infty)_{i\geq 1} \in \ell_p$, then [Cohen DeVore & Schwab]

$$d_m(K) \lesssim m^{-1/p+1}$$

- Towards general results [Devore et al. 2014]. Considering

$$\mathcal{A} = \{a(\cdot,\xi) : \xi \in \Xi\} \subset C(D),$$

then

$$d_m(K) \lesssim d_m(\mathcal{A})$$

How to construct (quasi-)optimal reduced spaces ?

- $u(\xi)$ is not directly accessible but solves

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

- Approximation $u_m(\xi)$ defined through Galerkin-type projections, such as

$$u_m(\xi) = \arg \min_{v \in V_m} \|A(v;\xi) - f\|$$

Under continuity and stability assumptions,

$$\|u(\xi) - u_m(\xi)\|_V \leq c \inf_{v \in V_m} \|u(\xi) - v\|_V \quad \text{(quasi-optimality)}$$

- Constructing optimal spaces is usually intractable $\longrightarrow$ suboptimal nested spaces (constructive approach)
  - Reduced Basis Method for $L^\infty(\Xi)$

$$V_m = span\{u(\xi^1), \ldots, u(\xi^m)\} \quad \text{with adaptive sampling}$$

  - Proper Generalized Decomposition for $L^2_\mu(\Xi)$

$$\inf_{\dim(V_m)=m} \int_\Xi \|A(u_m(\xi);\xi) - f\|^2 \mu(d\xi) \quad \text{subject to} \quad V_m \supset V_{m-1}$$

In summary

For the model reduction of parametric problems, we are able (in some situations) to

- quantify optimal model reduction
- provide a priori estimates for the performance
- propose algorithms that achieves quasi-optimality

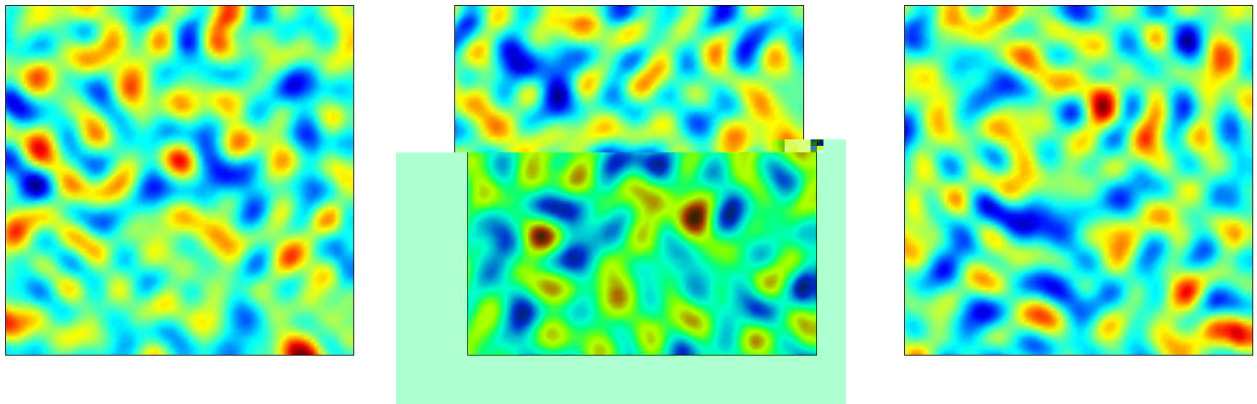
Outline

Examples of high dimensional problems in stochastic analyses

- Complex models with many uncertain parameters (geometry, source terms, constitutive laws)
- Random media with spatially correlated random fields

$$-\nabla \cdot (a \nabla u) = f \quad + \quad b.c.$$

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



Examples of high dimensional problems in stochastic analyses

- Stochastic differential equations:

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

  - Discretization of Wiener process $W_t \approx \sum_{k=1}^{d} \varphi_k(t)\xi_k$, and

$$X_t \approx X_t(\xi_1, \dots, \xi_d)$$

  - n-dimensional PDEs for probability density function

$$u(x_1, \dots, x_n, t)$$

    of X_t (Kolmogorov equation), or for functionals of X_t (Feynman-Kac formula)...

High-dimensional approximation

- Many problems requires the approximation (or integration) of high dimensional functions

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

- Classical discretization methods yields high-dimensional parametrizations

$$u(x_1, \ldots, x_d) \approx \sum_{i_1=1}^{n} \ldots \sum_{i_d=1}^{n} a_{i_1 \ldots i_d} \varphi_{i_1}^1(x_1) \ldots \varphi_{i_d}^d(x_d), \quad a \in \mathbb{R}^{n^d}$$

  - Number of parameters

$$N = n^d$$

  - Assuming $u \in C^s((0,1)^d)$, accuracy

$$\epsilon = O(n^{-s}) = O(N^{-s/d})$$

    and the number of parameters to achieve accuracy ϵ is

$$N = O(\epsilon^{-d/s}) \quad \text{(Curse of dimensionality)}$$

Curse of dimensionality - tractability

- Curse of dimensionality related to computational intractability in high dimension.
  - Quantitive definition through information-based complexity analysis
  - Tractability depends on the measure of precision and the available information.

- $N(\epsilon, d)$ being the number of linear informations to obtain a precision ϵ, intractability (curse of dimensionality) when

$$\lim_{\epsilon^{-1}+d \to \infty} \frac{\log N(\epsilon, d)}{\epsilon^{-1} + d} > 0$$

See [Novak,Wozniakowski]

Curse of dimensionality - tractability

- Weak tractability

$$\lim_{\epsilon^{-1}+d\to\infty} \frac{\log N(\epsilon, d)}{\epsilon^{-1} + d} = 0$$

- Polynomial tractability

$$N(\epsilon, d) \leq C\epsilon^{-p} d^q \quad \text{for all } \epsilon \text{ and } d$$

- Strong polynomial tractability

$$N(\epsilon, d) \leq C\epsilon^{-p} \quad \text{for all } \epsilon$$

Intractability for the approximation of smooth functions

Consider the set of functions

$$F_d = \left\{ u \in C^\infty((0,1)^d) : \sup_\alpha \|D^\alpha u\|_\infty < \infty \right\}$$

- Minimal approximation error using linear informations:

$$\epsilon(N,d) = \inf_{A_N} \sup_{u \in F_d} \|u - A_N(u)\|_\infty$$

  where the infimum is taken over all algorithms A_N using N linear informations on u and providing an approximation $A_N(u)$.
- Optimal rate of convergence is infinite: for arbitrary large s

$$\epsilon(N,d) = O(N^{-s}) \quad \text{as } N \to \infty$$

$$N(\epsilon,d) = O(\epsilon^{-1/s}) \quad \text{as } \epsilon \to 0$$

- But what about the constants in O ? [Novak 2009] proves

$$N(\epsilon,d) \geq 2^{\lfloor \frac{d}{2} \rfloor}$$

Curse of dimensionality !

Remedies: structured approximations

Order reduction methods must exploit specific structures (application dependent)

- Smoothness (anisotropy)
- Low effective dimensionality, e.g.

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

- Low-order interactions, e.g.

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

- Sparsity (relatively to a basis or frame)

$$u(x_1, \ldots, x_d) = \sum_{\alpha \in \Lambda} a_\alpha \psi_\alpha(x_1, \ldots, x_d) \approx \sum_{\alpha \in \Lambda_n \subset \Lambda} a_\alpha \psi_\alpha(x_1, \ldots, x_d)$$

- Low-rank structure

$$u(x_1, \ldots, x_d) \approx \sum_{i=1}^{r} u_{1,i}(x_1) \ldots u_{d,i}(x_d)$$

- ...

Outline

Sparse approximation

- We want to approximate a function $u \in L^p_\mu(\Xi; V)$. Consider a set of functions $\{\psi_\alpha; \alpha \in \Lambda\}$ (called a dictionary) whose span is dense in $L^p_\mu(\Xi)$, so that

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

  Typically, for multivariate functions

$$\psi_\alpha(\xi) = \psi^1_{\alpha_1}(\xi_1) \dots \psi^d_{\alpha_d}(\xi_d), \quad \Lambda = \{\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d; \sum_{i=1}^d \alpha_i < \infty\}$$

- 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:

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

- Sparse approximations can be obtained though interpolation, regression, Galerkin projections.

Best n-term approximation

The best n-term approximation in L^p norm is the solution of

$$\min_{\#\Lambda_n = n} \inf_{u_n \in X_{\Lambda_n}} \|u - u_n\|_p := \sigma_n^{(p)}(u)$$

where

$$X_{\Lambda_n} = \left\{ v = \sum_{\alpha \in \Lambda_n} v_\alpha \psi_\alpha ; v_\alpha \in V \right\}$$

Best n-term approximation

Questions:

- How fast $\sigma_n^{(p)}(u)$ converges to zero ?
  - If $(\|u_\alpha\|_V)_\alpha \in \ell^q$ and $(\psi_\alpha)_\alpha$ are orthonormal in L^2, then there exists Λ_n such that

$$\sigma_n^{(2)} \leq \min_{u_n \in X_{\Lambda_n}} \|u - u_n\|_2 \leq C n^{-s} \quad \text{with} \quad s = 1/q - 1/2$$

  - See  [Cohen-DeVore-Schwab 2010,Chkifa-Cohen-Schwab 2014] for a proof of $(\|u_\alpha\|_V)_\alpha \in \ell^p$ for a large class of parametric problems and for polynomial approximation. Results are working for infinitely many random variables.
- Selection of basis (or frame) suitable for a class of functions ?
- Best n-term approximation is a combinatorial problem. How to construct Λ_n in practice ?

Sparse approximation in practice

- A priori definition of the index set Λ_n, e.g. based on the properties of the class of functions we want to approximate (low-order interactions, anisotropy...). A priori error estimation can be useful.
  - $\Lambda_n = \{\alpha \in \mathbb{N}^d; \sum_{i=1}^d \alpha_i \leq p\}$
  - $\Lambda_n = \{\alpha \in \mathbb{N}^d; \sum_{i=1}^d \gamma_i \alpha_i \leq p\}$ (anisotropic)
  - $\Lambda_n = \{\alpha \in \mathbb{N}^d; f(\alpha) \leq p\}$.
- 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

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

Outline

Approximation of rank one functions

Consider the function $u : [0,1]^d \to \mathbb{R}$

$$u(x_1, \ldots, x_d) = u_1(x_1) \ldots u_d(x_d), \quad u_k \in C^s(0,1)$$

- Approximation of the factors

$$u_k(x_k) \approx \sum_{i=1}^{n} c_{k,i} \varphi_i(x_k) \quad \text{with error} \sim n^{-s}$$

- Number of parameters

$$N = dn$$

- Number of parameters to achieve accuracy ϵ

$$N(\epsilon, d) = O(d^{1+1/s} \epsilon^{-1/s})$$

Complexity of approximating rank-one tensors

- Consider the set of functions [Bachmayr 2013,Novak 2004]

$$F = \left\{ u(x_1, \ldots, x_d) = \prod_{i=1}^{d} u_i(x_i) : \|u_i\|_\infty \leq 1, \ \|u_i^{(s)}\|_\infty \leq M \right\}$$

  - If $M \geq 2^s s!$,

$$N(\epsilon, d) \geq 2^d \quad \text{for all } \epsilon < 1 \quad \text{(curse of dimensionality)}$$

  - Polynomial tractability (algorithm available) for the sets of functions

$$F^{x^*} = \{u \in F : u(x^*) \neq 0 \quad \text{for a known } x^*\}$$

$$F^V = \{u \in F : u \neq 0 \text{ on a box of measure greater than } V\}$$

Approximation with low-rank tensors (canonical format)

- Consider that function $u : [0,1]^d \to \mathbb{R}$ can be approximated with accuracy ϵ by an approximation with canonical rank $r(\epsilon)$:

$$u(x_1, \ldots, x_d) \approx \sum_{i=1}^{r(\epsilon)} u_{1,i}(x_1) \ldots u_{d,i}(x_d), \quad u_{k,i} \in C^s(0,1)$$

  - Approximation of each factor $u_{k,i}$ using n parameters with accuracy $\sim n^{-s}$
  - Number of parameters $N = r(\epsilon)nd$
  - Number of parameters to achieve accuracy ϵ

$$N(\epsilon, d) = O(r(\epsilon)^{1/s} d^{1+1/s} \epsilon^{-1/s})$$

- Do we beat the curse of dimensionality ?
  - What about $r(\epsilon)$ with respect to d ? some positive results...
  - Which information on u and which algorithm ?

Low-rank approximations

- Low-rank tensor subsets

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

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

- Canonical format has bad properties (non existence of best approximations, unstable format)
- Subspace based formats (Tucker or tree-based Tucker) have nice topological and geometrical properties (stability of best approximation, differentiable Banach manifolds)  [Falco-Hackbusch-Nouy 2014]
  - Existence of best approximations
  - Optimization on manifolds
  - Dynamical systems on manifolds (extension of Dirac-Frenkel theory to Banach tensor manifolds)

Operator equation in tensor format

$$A(u) = b \quad \text{with} \quad u \in X_{\|\cdot\|}, \quad X = \bigotimes_{\mu=1}^{d} V_\mu$$

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

Example: Laplace operator

$$A = \partial^2_{x_1} \otimes I \otimes \ldots \otimes I + \ldots + I \otimes \ldots \otimes I \otimes \partial^2_{x_d}$$

$$X = H^1_0(\Omega_1) \otimes \cdots \otimes H^1_0(\Omega_d)$$

Example: Parameter dependent operators (with affine decomposition)

$$A(\xi) = \sum_{i=1}^{m} A_i \lambda_i(\xi) \quad \text{or} \quad A = \sum_{i=1}^{m} A_i \otimes \Lambda_i$$

$$X = V \otimes L^p_\mu(\Xi)$$

Iterative solvers and low-rank tensor approximations

Given a low-rank format $\mathcal{M}_r$, replace standard iterations

$$u_n = B_n(u_{n-1})$$

with

$$u_n \in \mathcal{M}_{r_n} \quad \text{s.t.} \quad \|u_n - B_n(u_{n-1})\| \leq \epsilon$$

- 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

See e.g. [Kressner-Tobler 2010, Matthies-Zander 2011, Ballani-Grasedyck 2012, Bachmayr-Dahmen 2014,Giraldi-Nouy-Legrain 2014]

Direct approximation

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

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

by the optimization of a criterium

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

yielding a computable approximation of u in $\mathcal{M}$.

- 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:

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

Challenging issues

- Holy grail :
  - quantify optimal model order reduction : Information-based complexity
  - find algorithms achieving (quasi-)optimality
- Find suitable structures: sparsity, low-rank...
- Well-conditioned mathematical formulations for (quasi-)optimal model reduction
- Samples-based constructions: how to sample for a given approximation format ?
- Goal-oriented model order reduction: quantity of interest $Q(u)$, rare event computation, sensitivity analysis, inverse problems, ...
- Software. Minimize modifications of existing simulation codes.

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- **LOW-RANK FOR UQ AND PARAMETRIC MODELS**


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