High dimensional sparse polynomial approximations of parametric and stochastic PDE's

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with Ronald DeVore and Christoph Schwab
numerical results by Abdellah Chkifa

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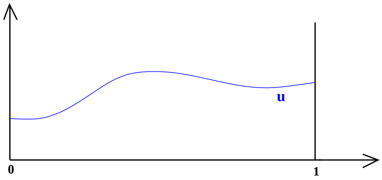

Error in terms of point spacing $h > 0$: if u has C^2 smoothness

$$\|u - R(u)\|_{L^\infty} \le C\|u''\|_{L^\infty} h^2.$$

Using piecewise polynomials of higher order, if u has C^m smoothness

$$\|u - R(u)\|_{L^\infty} \le C\|u^{(m)}\|_{L^\infty} h^m.$$

In terms of the number of samples $N \sim h^{-1}$, the error is estimated by N^{-m}.

In d dimensions : $u(y) = u(y_1, \cdots, y_d)$ with $y \in [0,1]^d$. With a uniform sampling, we still have

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but the number of samples is now $N \sim h^{-d}$, and the error estimate is in $N^{-m/d}$.

The curse of dimensionality

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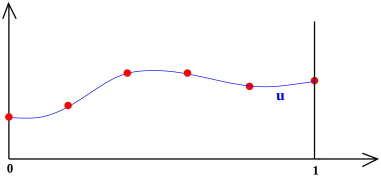

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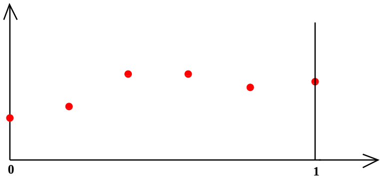

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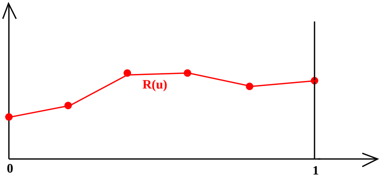

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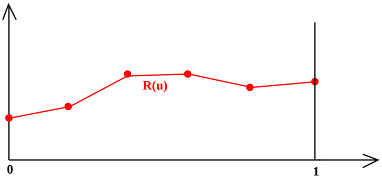

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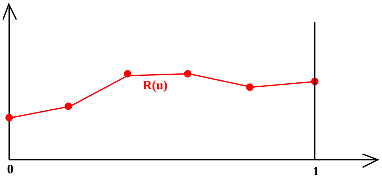

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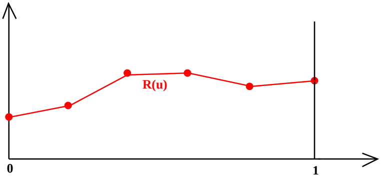

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Can be explained by nonlinear manifold width (DeVore-Howard-Micchelli).

Let X be a normed space and $\mathcal{K} \subset X$ a compact set.

Consider maps $E : \mathcal{K} \mapsto \mathbb{R}^N$ (encoding) and $R : \mathbb{R}^N \mapsto X$ (reconstruction).

Introducing the distorsion of the pair (E, R) over $\mathcal{K}$

$$\max_{u \in \mathcal{K}} \|u - R(E(u))\|_X,$$

we define the nonlinear N-width of $\mathcal{K}$ as

$$d_N(\mathcal{K}) := \inf_{E,R} \max_{u \in \mathcal{K}} \|u - R(E(u))\|_X,$$

where the infimum is taken over all continuous maps (E, R).

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High dimensional problems occur frequently

PDE's with solutions $u(x,v,t)$ defined in phase space : $d=7$.

Post-processing of numerical codes : u solver with imput parameters $(y_1,\cdots,y_d)$.

Learning theory : u regression function of imput parameters $(y_1,\cdots,y_d)$

In these applications d may be of the order up to 10^3.

Approximation of stochastic-parametric PDEs (this talk) : $d=+\infty$.

Smoothness properties of functions should be revisited by other means than C^m classes, and appropriate approximation tools should be used.

Key ingredients :

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(ii) Variable reduction

(iii) Anisotropy

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A model elliptic PDE

We consider the steady state diffusion equation

$$-\mathrm{div}(a\nabla u) = f \ \text{ in } \ D \subset \mathbb{R}^m \ \text{ and } \ u = 0 \ \text{ on } \ \partial D,$$

where $f = f(x) \in L^2(D)$ and $a = a(x,y)$ are variable coefficients depending on $x \in D$ and on a vector y of parameters in an affine manner :

$$a = a(x,y) = \bar{a}(x) + \sum_{j>0} y_j \psi_j(x), \ \ x \in D, y = (y_j)_{j>0} \in U := [-1,1]^{\mathbb{N}},$$

where $(\psi_j)_{j>0}$ is a given family of functions.

The parameters may be deterministic (control, optimization) or random (uncertainty modeling and propagation, reliability assessment).

Uniform ellipticity assumption :

$$(UEA) \qquad 0 < r \le a(x,y) \le R, \ \ x \in D, \ y \in U.$$

Then $u : y \mapsto u(y) = u(\cdot, y)$ is a bounded map from U to $V := H_0^1(\Omega)$:

$$\|u(y)\|_V \le C_0 := \frac{\|f\|_{V^*}}{r}, \ \ y \in U, \ \text{ where } \ \|v\|_V := \|\nabla v\|_{L^2}.$$

Proof : multiply equation by u and integrate

$$r\|u\|_V^2 \le \int_D a\nabla u \cdot \nabla u = -\int_D u\,\mathrm{div}(a\nabla u) = \int_D uf \le \|u\|_V \|f\|_{V^*}.$$

Objective : build a computable approximation to this map at reasonable cost, i.e. simultaneaously approximate $u(y)$ for all $y \in U$.

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Polynomial expansions

Use of multivariate polynomials in the y variable.

Sometimes referred to as "polynomial chaos" in the random setting (Ghanem-Spanos, Babushka-Tempone-Nobile-Zouharis, Karniadakis, Schwab...).

We study the convergence of the Taylor development

$$u(y) = \sum_{\nu \in \mathcal{F}} t_\nu y^\nu,$$

where

$$y^\nu := \prod_{j>0} y_j^{\nu_j}.$$

Here $\mathcal{F}$ is the set of all finitely supported sequences $\nu = (\nu_j)_{j>0}$ of integers (only finitely many ν_j are non-zero). The Taylor coefficients $t_\nu \in V$ are

$$t_\nu := \frac{1}{\nu!} \partial^\nu u_{|y=0} \;\; \text{with} \;\; \nu! := \prod_{j>0} \nu_j! \;\; \text{and} \;\; 0! := 1.$$

We also studied Legendre series $u(y) = \sum_{\nu \in \mathcal{F}} u_\nu L_\nu$ where $L_\nu(y) := \prod_{j>0} L_{\nu_j}(y_j)$.

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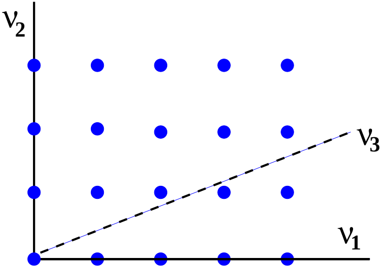


Objective : identify a set $\Lambda \subset \mathcal{F}$ with $\#(\Lambda) \leq N$ such that u is well approximated in the space

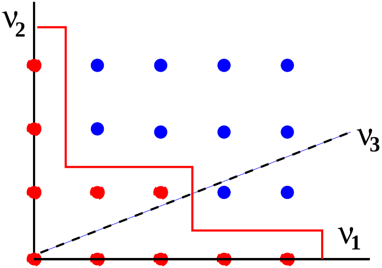
$$V_\Lambda := \{\sum_{\nu\in\Lambda} c_\nu y^\nu \ ; \ u_\nu \in V\},$$

for example by the partial Taylor expansion

$$u_\Lambda(y) := \sum_{\nu\in\Lambda} t_\nu y^\nu .$$

Sparse N-term polynomial approximation

The sequence $(t_\nu)_{\nu\in\mathcal{F}}$ is indexed by countably many integers.



Objective : identify a set $\Lambda\subset\mathcal{F}$ with $\#(\Lambda)\leq N$ such that u is well approximated in the space

$$V_\Lambda := \{\sum_{\nu\in\Lambda} c_\nu y^\nu \ ; \ u_\nu \in V\},$$

for example by the partial Taylor expansion

$$u_\Lambda(y) := \sum_{\nu\in\Lambda} t_\nu y^\nu .$$

A-priori choices for Λ have been proposed : (anisotropic) sparse grid defined by restrictions of the type $\sum_j \alpha_j \nu_j \leq A(N)$ or $\prod_j (1+\beta_j \nu_j) \leq B(N)$.

Instead we want study a choice of Λ optimally adapted to u.

For all $y \in U = [-1,1]^{\mathbb{N}}$ we have

$$\|u(y) - u_\Lambda(y)\|_V \leq \|\sum_{\nu \notin \Lambda} t_\nu y^\nu\|_V \leq \sum_{\nu \notin \Lambda} \|t_\nu\|_V$$

Best N-term approximation in the $\ell^1(\mathcal{F})$ norm : use for Λ the N largest $\|t_\nu\|_V$.

Observation (Stechkin) : if $(\|t_\nu\|_V)_{\nu \in \mathcal{F}} \in \ell^p(\mathcal{F})$ for some $p < 1$, then for this Λ,

$$\sum_{\nu \notin \Lambda} \|t_\nu\|_V \leq CN^{-s}, \quad s := \frac{1}{p} - 1, \quad C := \|(\|t_\nu\|_V)\|_p.$$

Proof : with $(t_n)_{n>0}$ the decreasing rearrangement, we combine

$$\sum_{\nu \notin \Lambda} \|t_\nu\|_V = \sum_{n>N} t_n = \sum_{n>N} t_n^{1-p} t_n^p \leq t_N^{1-p} C^p \quad \text{and} \quad N t_N^p \leq \sum_{n=1}^{N} t_n^p \leq C^p.$$

Question : do we have $(\|t_\nu\|_V)_{\nu \in \mathcal{F}} \in \ell^p(\mathcal{F})$ for some $p < 1$?

Best N-term approximation

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The main result

Theorem (Cohen-DeVore-Schwab, 2009) : under the uniform ellipticity assumption (UAE), then for any $p < 1$,

$$(\|\psi_j\|_{L^\infty})_{j\geq 0} \in \ell^p(\mathbb{N}) \Rightarrow (\|t_\nu\|_V)_{\nu\in\mathcal{F}} \in \ell^p(\mathcal{F}).$$

Interpretations :

(i) The Taylor expansion of $u(y)$ inherits the sparsity properties of the expansion of $a(y)$ into the ψ_j.

(ii) We approximate $u(y)$ in $L^\infty(U)$ with algebraic rate N^{-s} despite the curse of (infinite) dimensionality, due to the fact that y_j is less influencial as j gets large.

(iii) The set $\mathcal{K} := \{u(y)\ ;\ y \in U\}$ is compact in V and has small N-width $d_N(\mathcal{K}) := \inf_{\dim(E)\leq N} \max_{v\in\mathcal{K}} \operatorname{dist}(v, E)_V$: for all y

$$u_\Lambda(y) := \sum_{\nu\in\Lambda} t_\nu y^\nu = \sum_{\nu\in\Lambda} y^\nu t_\nu \ \in E_\Lambda := \mathrm{Span}\{t_\nu\ ;\ \nu \in \Lambda\}.$$

With Λ corresponding to the N largest $\|t_\nu\|_V$, we find that

$$d_N(\mathcal{K}) \leq \max_{y\in U} \operatorname{dist}(u(y), E_\Lambda)_V \leq \max_{y\in U} \|u(y) - u_\Lambda(y)\|_V \leq CN^{-s}.$$

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Estimates on $\|t_\nu\|_V$ by complex analysis : extend $u(y)$ to $u(z)$ with $z=(z_j)\in\mathbb{C}^{\mathbb{N}}$.

Uniform ellipticity $0<r\leq\overline{a}(x)+\sum_{j>0}y_j\psi_j(x)$ for all $x\in D, y\in U$ is equivalent to

$$\sum_{j>0}|\psi_j(x)|\leq\overline{a}(x)-r,\ \ x\in D.$$

This allows to say that with $a(x,z)=\overline{a}(x)+\sum_{j>0}z_j\psi_j(x)$,

$$0<r\leq\Re(a(x,z))\leq|a(x,z)|\leq 2R,$$

for all $z\in\mathcal{U}:=\{|z|\leq 1\}^{\mathbb{N}}=\otimes\{|z_j|\leq 1\}$.

Lax-Milgram theory applies : $\|u(z)\|\leq C_0=\frac{\|f\|_{V^*}}{r}$ for all $z\in\mathcal{U}$. The function $u\mapsto u(z)$ is holomorphic in each variable z_j at any $z\in\mathcal{U}$.

Extended domains of holomorphy : if $\rho=(\rho_j)_{j\geq 0}$ is any positive sequence such that for some $\delta>0$

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$$u(z) = \frac{1}{2i\pi} \int_{|z'|=a} \frac{u(z')}{z - z'} dz',$$

which leads by m differentiation at $z = 0$ to $|u^{(m)}(0)| \leq m! a^{-m} \max_{|z| \leq a} |u(z)|$.

Recursive application of this to all variables z_j such that $\nu_j \neq 0$, with $a = \rho_j$, for a δ-admissible sequence ρ gives

$$\|\partial^\nu u_{|z=0}\|_V \leq C_\delta \nu! \prod_{j>0} \rho_j^{-\nu_j}.$$

and therefore

$$\|t_\nu\|_V \leq C_\delta \prod_{j>0} \rho_j^{-\nu_j} = C_0 \rho^{-\nu}.$$

Since ρ is not fixed we have

$$\|t_\nu\|_V \leq C_\delta \inf\{\rho^{-\nu} \;\; ; \;\; \rho \text{ is } \delta-\text{admissible}\}.$$

We do not know the general solution to this problem, except when the ψ_j have disjoint supports. Instead design a particular choice $\rho = \rho(\nu)$ of δ-admissible sequences with $\delta = r/2$, for which we prove that

$$(\|\psi_j\|_{L^\infty})_{j \geq 0} \in \ell^p(\mathbb{N}) \Rightarrow (\rho(\nu)^{-\nu})_{\nu \in \mathcal{F}} \in \ell^p(\mathcal{F}).$$

Estimate on the Taylor coefficients

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A simple case

Assume that the ψ_j have disjoint supports. Then we maximize separately the ρ_j so that

$$\sum_{j>0} \rho_j |\psi_j(x)| \leq \overline{a}(x) - \frac{r}{2}, \quad x \in D,$$

which leads to

$$\rho_j := \min_{x \in D} \frac{\overline{a}(x) - \frac{r}{2}}{|\psi_j(x)|}.$$

We have

$$\|t_\nu\|_V \leq 2C_0 \rho^{-\nu} = 2C_0 b^\nu,$$

where $b = (b_j)$ and

$$b_j := \rho_j^{-1} = \frac{|\psi_j(x)|}{\overline{a}(x) - \frac{r}{2}} \leq \frac{\|\psi_j\|_{L^\infty}}{R - \frac{r}{2}}.$$

Therefore $b \in \ell^p(\mathbb{N})$. From (UEA), we have $|\psi_j(x)| \leq \overline{a}(x) - r$ and thus $\|b\|_{\ell^\infty} < 1$.

We finally observe that

$$b \in \ell^p(\mathbb{N}) \text{ and } \|b\|_{\ell^\infty} < 1 \Leftrightarrow (b^\nu)_{\nu \in \mathcal{F}} \in \ell^p(\mathcal{F}).$$

Proof : factorize

$$\sum_{\nu \in \mathcal{F}} b^{p\nu} = \prod_{j>0} \sum_{n \geq 0} b_j^{pn} = \prod_{j>0} \frac{1}{1 - b_j^p}.$$

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$$b \in \ell^p(\mathbb{N}) \ \text{ and } \ \|b\|_{\ell^\infty} < 1 \Leftrightarrow (b^\nu)_{\nu \in \mathcal{F}} \in \ell^p(\mathcal{F}).$$

Proof : factorize

$$\sum_{\nu \in \mathcal{F}} b^{p\nu} = \prod_{j>0} \sum_{n \ge 0} b_j^{pn} = \prod_{j>0} \frac{1}{1 - b_j^p}.$$

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Recursive computation of the Taylor coefficients : with e_j the Kroenecker sequence

$$\int_D \bar{a}\nabla t_\nu \nabla v = -\sum_{j:\ \nu_j \neq 0} \int_D \psi_j \nabla t_{\nu - e_j} \nabla v, \ \ v \in V.$$

We compute the t_ν on sets Λ with monotone structure : $\nu \in \Lambda$ and $\mu \leq \nu \Rightarrow \mu \in \Lambda$.

Given such a Λ_k and the $(t_\nu)_{\nu \in \Lambda_k}$ we compute the t_ν for ν in the margin

$$\mathcal{M}_k := \{\nu \notin \Lambda_k \, ; \, \nu - e_j \in \Lambda_k \ \text{ for some } j\},$$

and build the new set by bulk search : $\Lambda_{k+1} = \Lambda_k \cup \mathcal{S}_k$, with $\mathcal{S}_k \subset \mathcal{M}_k$ smallest such that $\sum_{\nu \in \mathcal{S}_k} \|t_\nu\|_V^2 \geq \theta \sum_{\nu \in \mathcal{M}_k} \|t_\nu\|_V^2$, with $\theta \in (0,1)$.

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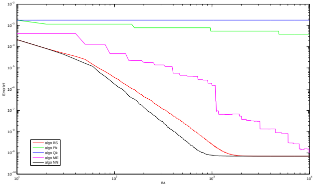
Test case in moderate dimension $d = 16$

Physical domain $D = [0,1]^2 = \cup_{j=1}^{d} D_j$.

Diffusion coefficients $a(x,y) = 1 + \sum_{j=1}^{d} y_j \left(\frac{0.9}{j^2}\right) \chi_{D_j}$.

Adaptive search of Λ implemented in C++, spatial discretization by FreeFem++.

Comparison between the Λ_k generated by the adaptive algorithm (red) and non-adaptive choices $\{\sup \nu_j \leq k\}$ (blue) or $\{\sum \nu_j \leq k\}$ (green) or k largest a-priori bounds on the $\|t_\nu\|_V$ (pink)



Highest polynomial degree with $\#(\Lambda) = 1000$ coefficients : 1, 4, 115 and 81.

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First numerical results in moderate dimensionality : reveal the adavantages of an adaptive approach. Goal : implementation for very high or infinite dimensionality.

Many applications in engineering.

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