From linear to nonlinear n-width: optimality in reduced modelling

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IHP, 08-11-2021



Announcing two great conferences, hopefully in physical format

1. Curves and Surfaces: Arcachon, France, June 20-24, 2022

Registration open: cs2022.sciencesconf.org

Foundation of Computational Mathematics: Whistler, Canada, June 12-21, 2023.
 Registration opening should be officially announced in coming months.

Save the dates!

Agenda

- 1. Linear widths
- 2. Widths of parametrized PDEs and reduced bases
- 3. Nonlinear widths
- 4. Widths and sampling numbers

Kolmogorov linear n-width

We are interested in approximating general functions $u \in V$, where V is a Banach space, by simpler functions v picked from a linear subspace $V_n \subset V$ of finite dimension n.

Classical Banach spaces : Lebesgue $L^p(\Omega)$, Sobolev $W^{m,p}(\Omega)$ for $\Omega \subset \mathbb{R}^d$.

Classical linear subspaces : algebraic or trigonometric polynomials of some prescribed degree, splines or finite elements on some given mesh, span of the n first elements $\{e_1, \ldots, e_n\}$ from a given basis $(e_k)_{k>1}$ of V.

Model class reflecting the properties the target function : $u \in \mathcal{K}$, where \mathcal{K} is a compact set of V. In parametrized PDEs, the set \mathcal{K} is the solution manifold that gathers all solutions $u(y) \in V$ as the parameter vector y varies.

Best choice of approximation spaces for this model class?

The space V_n approximate \mathcal{K} with uniform accuracy

$$\operatorname{dist}(\mathcal{K}, V_n)_V := \max_{u \in \mathcal{K}} \min_{v \in V_n} \|u - v\|_V$$

A.N. Kolmogorov (1936) defines the linear *n*-width of $\mathcal K$ in the metric V as

$$d_n(\mathcal{K})_V := \inf_{\dim(V_n) = n} \operatorname{dist}(\mathcal{K}, V_n)_V$$

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Intuition



The optimal space achieving the infimum in

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An analog concept in the stochastic framework: PCA

Assume that V is a Hilbert space and u is a random variable taking its value in V. Optimal spaces in the mean-square sense.

$$\kappa_n^2 = \kappa_n(u)_V^2 := \min_{\dim(V_n) = n} \mathbb{E}\Big(\|u - P_{V_n}u\|_V^2\Big).$$

The space achieving the minimum is easily characterized by principal component analysis: consider the covariance operator

$$v \mapsto Rv = \mathbb{E}(\langle u, v \rangle u),$$

which is compact, when assuming that $\mathbb{E}(\|u\|_V^2) < \infty$. Diagonalized in the Karhunen-Loeve basis $(\varphi_k)_{k \geq 1}$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \rightarrow 0$.

Then $V_n := \operatorname{span}\{\varphi_1, \dots, \varphi_n\}$ and $\kappa_n^2 = \sum_{k > n} \lambda_k$.

Note that $\kappa_n(u)_V^2 \leq d_n(\mathcal{K})_V^2$ when u is supported in \mathcal{K} .

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Variants to *n*-width : realization of the approximation

The best approximation $u_n = \operatorname{argmin}\{\|u - v\|_V : v \in V_n\}$ is the orthogonal projection if V is a Hilbert space.

For a general Banach space, the map $u \mapsto u_n$ is not linear, and may even not be continuous (non-uniqueness of best approximation).

This motivates alternate definitions of widths where we impose linearity or continuity of the approximation process.

Approximation numbers are defined as

$$a_n(\mathcal{K})_V := \inf_{L} \max_{u \in \mathcal{K}} \|u - Lu\|_V,$$

with infimum taken over all linear maps L such that $rank(L) \leq n$.

In a general Banach space $d_n \leq a_n \leq \sqrt{n}d_n$ and right equality may hold

On the other hand one can prove that

$$d_n(\mathcal{K})_V := \inf_F \max_{u \in \mathcal{K}} \|u - F(u)\|_V,$$

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Behaviour of *n*-widths of smoothness classes

Typical compact sets in $V=L^p(\Omega)$ are balls of smoothness spaces. The behaviour of n-width is well understood for such sets. Example : $V=L^\infty(I)$ where $I=[0,1]\subset \mathbb{R}$

and

$$\mathcal{K} = \mathcal{U}(\operatorname{Lip}(I)) = \{u : \max\{\|u\|_{L^{\infty}}, \|u'\|_{L^{\infty}}\} \le 1\},$$

Then one can prove

$$d_n(\mathcal{K})_V = \frac{1}{2n}, \quad n \geq 1,.$$

More generally when $V=W^{t,p}(\Omega)$ for some bounded Lipschitz domain $\Omega\subset\mathbb{R}^d$ and \mathcal{K} is the unit ball of $W^{s,p}(\Omega)$ with s>t, one can prove

$$cn^{-(s-t)/d} \le d_n(\mathcal{K})_V \le Cn^{-(s-t)/d}, \quad n \ge 1.$$

Curse of dimensionality: exponential growth in d of the needed n to reach accuracy ε .

Proof of upper bound : use a standard approximation method (piecewise polynomials, finite elements, or splines, on uniform partitions of Ω)

Proof of lower bound? Two systematic approaches.

Bernstein width

Lemma : let $B_W = \{u \in W : ||u||_V \le 1\}$ be the unit ball of a subspace $W \subset V$ of dimension n+1, then $\frac{d_n(B_W)_V}{d_n(B_W)_V} = 1$.

Proof : trivial if V is a Hilbert space. Follows from Borsuk-Ulam antipodality theorem in the Banach space case : for any continuous application F from an n-sphere $S_n = \partial B_W$ to an n dimensional space V_n , there exists $x \in S_n$ such that F(x) = F(-x).

It follows that $d_n(\mathcal{K})_V \ge r$ if \mathcal{K} contains the rescaled ball rB_W of an n+1-dimensional space W. In other words

$$d_n(\mathcal{K})_V \geq b_n(\mathcal{K})_V, \quad n \geq 1,$$

where the Bernstein n-width $b_n(\mathcal{K})_V$ is defined as the largest $r\geq 0$ such that there exists $W\subset V$ of dimension n+1 with $rB_W\subset \mathcal{K}$.

Bernstein width

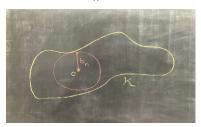
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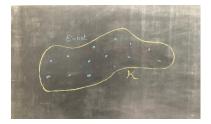
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Entropy numbers

Define $\varepsilon_n(\mathcal{K})_V$ as the smallest ε such that \mathcal{K} can be covered by 2^n balls of radius ε :

$$\mathcal{K} \subset \bigcup_{i=1,\ldots,2^n} B(u^i,\varepsilon), \qquad B(u^i,\varepsilon) := \{u \,:\, \|u-u^i\|_V \leq \varepsilon\}.$$



Related to lossy coding: Elements of K can be encoded with n bits up to precision ε_n .

Carl's inequality : for all s > 0 one has

$$(n+1)^s \varepsilon_n(\mathcal{K})_V \leq C_s \sup_{m=0,\ldots,n} (m+1)^s d_m(\mathcal{K})_V, \quad n \geq 0$$

In particular

$$d_n(\mathcal{K})_V \leq n^{-s}, \quad n \geq 0 \implies \varepsilon_n(\mathcal{K})_V \leq n^{-s}, \quad n \geq 0.$$

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$$d_n(\mathcal{K})_V \lesssim n^{-s}, \quad n \geq 0 \implies \varepsilon_n(\mathcal{K})_V \lesssim n^{-s}, \quad n \geq 0.$$

Reduced modeling for parametrized PDEs

Complex problems are often modelled by PDEs involving several physical parameters $y=(y^1,\ldots,y^d)\in Y\subset\mathbb{R}^d$.

$$\mathcal{P}(u, y) = 0$$
,

For each $y \in Y$, we assume well-posedness and therefore existence of a unique solution $u(y) \in V$.

In certain applications (optimization, inverse problems, uncertainty quantification), we may need to solve $y\mapsto u(y)$ for many instances of $y\in Y$: requires computational methods that are uniformly cheap and efficient, uniformly over $y\in Y$.

We are interested in well approximating the solution manifold

$$\mathcal{K} := \{ u(y) : y \in Y \} \subset V,$$

which we assume to be compact.

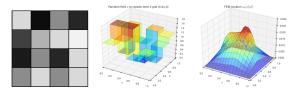
Reduced modeling usually involves two steps:

- 1. In a (costly) offline stage, we search for spaces V_n of dimension n that approximate as best as possible the set \mathcal{K} (benchmark $d_n(\mathcal{K})_V$). These spaces are quite different from classical finite element spaces.
- 2. In a (cheap) online stage, for any required $y \in Y$ we may compute an accurate approximation $u_n(y) \in V_n$ of u(y), for example by the Galerkin method.

An instructive example : consider the steady-state diffusion equation

$$-\operatorname{div}(a\nabla u)=f,$$

on a 2d domain Ω (+ boundary conditions), with piecewise constant diffusion function a=a(y) having value $\overline{a}+y_j$ on subdomain Ω_j , where $y=(y_1,\ldots,y_d)\in Y=[-c,c]^d$.



How large is the *n*-width of $\mathcal{K} = \{u(y) : y \in Y\} \subset V = H^1(\Omega)$?

Solutions u(y) are bounded in H^s iff s < 3/2 and $d_n(\mathcal{U}(H^s))_{H^1} \sim n^{-(s-1)/2} \gtrsim n^{-1/4}$.

In fact $d_n(\mathcal{K})_{H^1}$ decreases faster than $\mathcal{O}(\exp(-cn^{1/d}))$: approximate by power series

$$\max_{y \in Y} \left\| u(y) - \sum_{|v| \le k} u_v y^v \right\|_{H^1} \le C \exp(-ck), \quad y^v = y_1^{v_1} \dots y_d^{v_d},$$

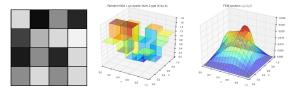
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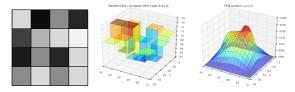
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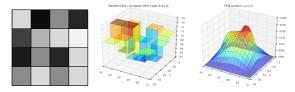
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A general result for infinite dimensional parameter dependence

Theorem (Cohen-DeVore, 2016) : Let V_1 and V_2 be two complex valued Banach spaces and $\mathcal{K}_1 \subset V_1$ be a compact set. Let

$$F: V_1 \rightarrow V_2$$

be a map that is holomorphic on an open neighbourhood of \mathcal{K}_1 . Then, with $\mathcal{K}_2 := F(\mathcal{K}_1)$, one has for all s > 1

$$\sup_{n\geq 0} n^s d_n(\mathcal{K}_1)_{V_1} < \infty \implies \sup_{n\geq 0} n^t d_n(\mathcal{K}_2)_{V_2} < \infty, \quad t < s-1.$$

Note that if F was a continuous linear map, one would simply have

$$d_n(\mathcal{K}_2)_{V_2} \leq C d_n(\mathcal{K}_1)_{V_1}, \quad C = ||F||_{V_1 \to V_2}.$$

The proof goes by expanding $a \in \mathcal{K}_1$ in a suitable basis $a = a(y) = \sum_{j \ge 1} y_j \psi_j$ with decay properties on the $\|\psi_j\|_{V_1}$ and then approximate F(a(y)) by polynomials in y. This induces a loss of 1 in the rate of decay. Open problem: same rate t = s?

This result applies to elliptic equations such as $-\text{div}(a\nabla u)=f$ for the map $F:a\to u$ with $V_1=L^\infty$ and $V_2=H^1$. Also applies to parabolic equations, nonlinear problems such as Navier-Stokes equations, and to these problems set on parametrized domains. It does not apply to hyperbolic equations.

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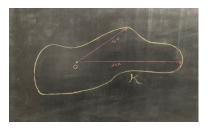
The reduced basis algorithm

Idea : use particular instances $u^i = u(y^i) \in \mathcal{K}$ for generating $V_n = \operatorname{span}\{u^1, \dots, u^n\}$.

Greedy selection in offline stage : having generated u^1, \dots, u^{k-1} , select next instance

$$||u^k - P_{V_{k-1}}u^k||_V = \max_{u \in \mathcal{K}} ||u - P_{V_{k-1}}u||_V,$$

where $P_{V_{k-1}}$ is the orthogonal projection. Here we assume V to be a Hilbert space.



In practice, weak selection $\|u - P_{V_{k-1}}u^k\|_V \ge \gamma \max_{u \in \mathcal{K}} \|u - P_{V_{k-1}}u\|_V$, for fixed $\gamma \in]0,1[$, and maximization on a large finite training set $\widetilde{\mathcal{K}} \subset \mathcal{K}$.

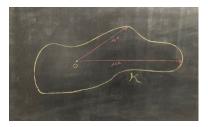
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In practice, weak selection $\|u - P_{V_{k-1}}u^k\|_V \ge \gamma \max_{u \in \mathcal{K}} \|u - P_{V_{k-1}}u\|_V$, for fixed $\gamma \in]0,1[$, and maximization on a large finite training set $\widetilde{\mathcal{K}} \subset \mathcal{K}$.

Approximation performances

For the greedily generated spaces V_n , we would like to compare

$$\sigma_n(\mathcal{K})_{\mathit{V}} = \operatorname{dist}(\mathcal{K}, \mathit{V}_n)_{\mathit{V}} = \max_{\mathit{u} \in \mathcal{K}} \|\mathit{u} - \mathit{P}_{\mathit{V}_n} \mathit{u}\|_{\mathit{V}},$$

with the *n*-widths $d_n(\mathcal{K})_V$ that correspond to the optimal spaces.

Direct comparison is deceiving

Buffa-Maday-Patera-Turinici (2010) : $\sigma_n \leq n2^n d_n$.

For all $n \geq 0$ and $\varepsilon > 0$, there exists \mathcal{K} such that $\sigma_n(\mathcal{K})_V \geq (1 - \varepsilon)2^n d_n(\mathcal{K})_V$

Comparison is much more favorable in terms of convergence rate.

Theorem (Binev-Cohen-Dahmen-DeVore-Petrova-Wojtaszczyk, 2013) : For any s>0

$$\sup_{n\geq 1} \mathsf{n}^{\mathsf{s}} \mathsf{d}_n(\mathcal{K})_V < \infty \Rightarrow \sup_{n\geq 1} \mathsf{n}^{\mathsf{s}} \sigma_n(\mathcal{K})_V < \infty,$$

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Failure of linear reduced modeling

Linear reduced modeling for parametrized hyperbolic PDEs suffers from a slow decay of Kolmogorov n-width.

Simple example: consider the univariate linear transport equation

$$\partial_t u + a \partial_x u = 0$$
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with constant velocity $a \in \mathbb{R}$ and initial condition $u_0 = u(x, 0) = \chi_{[0,1]}(x)$.

Parametrize the solution by the velocity $a \in [a_{\min}, a_{\max}]$ and consider the solution manifold at final time T = 1.

$$\mathcal{H} = \{\chi_{[a,a+1]} : a \in [a_{\mathsf{min}}, a_{\mathsf{max}}]\}.$$

It can be proved that for 1

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Nonlinear approximation

For such problems, one expects improved performance by nonlinear methods.

Non-linear approximation : the function u is approximated by simpler function $v \in \Sigma_n$ that can be described by $\mathcal{O}(n)$ parameters, however Σ_n is not a linear space.

- Rational fractions : $\Sigma_n = \left\{ rac{p}{q} \, ; \, p,q \in \mathbb{P}_n
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- Best *n*-term / sparse approximation in a basis $(e_k)_{k\geq 1}$: pick approximation from the set $\Sigma_n = \{\sum_{k\in F} c_k e_k : \#(E) \leq n\}$.
- Piecewise polynomials, splines, finite elements on meshes generated after *n* step of adaptive refinement (select and split an element in the current partition).
- Neural networks : functions $v: \mathbb{R}^d \to \mathbb{R}^m$ of the form

$$v = A_k \circ \sigma \circ A_{k-1} \circ \sigma \circ A_{k-2} \circ \cdots \circ \sigma \circ A_1,$$

where $A_j: \mathbb{R}^{d_j} \to \mathbb{R}^{d_{j+1}}$ is affine and σ is a nonlinear (rectifier) function applied componentwise, for example $\sigma(x) = RELU(x) = \max\{x,0\}$. Here Σ_n is the set of such functions when the total number of parameters does not exceed n.

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Library widths

A library \mathcal{L}_n is a finite collection of linear spaces $V_n \subset V$ of dimension at most n.

We approximate u by picking a space from \mathcal{L}_n , resulting in the error

$$e(u,\mathcal{L}_n)_V = \min_{V_n \in \mathcal{L}_n} \min_{v \in V_n} \|u - v\|_V.$$

Temlyakov (1998) defines the library width

$$d_{N,n}(\mathcal{K})_V := \inf_{\#(\mathcal{L}_n) \le N} \max_{u \in \mathcal{K}} e(u, \mathcal{L}_n)_V.$$

Note that $d_{1,n} = d_n$

The interesting regime is when N >> n. Typical choices that have been studied are $N = A^n$ or $N = n^{an}$ for some A > 1 or a > 0.

Remark: optimal library approximation amounts in splitting the set \mathcal{K} into N different component \mathcal{K}_j , each of them being approximated by some optimal n-dimensional space V_n^j picked from the library.

This type of width is well adapted to describe optimality for best *n*-term approximation or adaptive refinements, but not for neural networks or rational fractions.

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Manifold widths

Naive idea : replace linear spaces V_n of dimension n by smooth manifolds \mathcal{M}_n of dimension n in the definition of d_n .

This would lead to the quantity

$$\inf_{\dim(\mathcal{M}_n)=n} \max_{u \in \mathcal{K}} \min_{v \in V} \|u-v\|_V,$$

However its value is 0 even for n=1 : space filling curves!

DeVore-Howard-Michelli (1989): impose continuous selection by defining

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Both library and manifold widths match known rates of nonlinear approximation (DeVore-Popov, 1980-1990's) by wavelets or adaptive finite elements : if $V=L^p(\Omega)$ and $\mathcal{K}=\mathcal{U}(B^s_{q,q}(\Omega))$ for $\frac{1}{q}<\frac{1}{p}+\frac{s}{d}$, one has

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Upper bounds obtained by these classical nonlinear approximation results.

Library widths satisfy Carl's inequality (for the regimes $N = A^n$ or $N = n^{an}$)

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Manifold widths do not satisty Carl's inequality but are bounded by below by Bernstein widths (by the Borsuk-Ulam argument).

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Cohen-DeVore-Petrova-Wojtaszczyk (2020) : for some fixed L>1 define

$$\delta_{n,L}(\mathcal{K})_{V} := \inf_{D,E} \max_{u \in \mathcal{K}} \|u - D(E(u))\|_{V},$$

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Stable widths and entropies

When V is a Hilbert space, stable widths are strongly tied to entropy numbers.

Theorem : Let V be a Hilbert space, then for any L>1, there exists a constant c=c(L) such that, for any compact set \mathcal{K} ,

$$\delta_{cn,L}(\mathcal{K})_V \leq 3\varepsilon_n(\mathcal{K})_V$$
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With L=2 one can take c=26.

Together with Carl's inequality, this means that

$$\sup_{n\geq 0} n^{\mathfrak s} \delta_{n,L}(\mathcal K)_{V} < \infty \iff \sup_{n\geq 0} n^{\mathfrak s} \epsilon_{n}(\mathcal K)_{V} < \infty,$$

for all s > 0.

We do not know if this result holds for Banach spaces. Proof for Hilbert spaces

- 1. Consider \mathcal{N} an ε_n -net of \mathcal{K} with $\#(\mathcal{N}) = 2^n$
- 2. Johnson-Lindenstrauss projection as encoder : $E = P_W$ where $\dim(W) \leq cn$

$$L^{-1}\|u^i - u^j\|_V \le \|P_W(u^i - u^j)\|_V \le \|u^i - u^j\|_V, \quad u^i, u^j \in \mathcal{N}.$$

- 3. This gives an exact decoding map that is L-Lipschitz from $P_W \mathcal{N}$ to \mathcal{N}
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Stable width of solution manifolds

For the linear transport equation manifold $\mathcal{H}=\left\{\chi_{[a,a+1]}:a\in[a_{\min},a_{\max}]\right\}$ it is easily established that entropy numbers in L^p spaces have exponential decay

$$\varepsilon_n(\mathcal{H})_{L^p} \leq C \exp(-cn), \quad n \geq 0.$$

This implies in particular that $\delta_{n,L}(\mathcal{H})_{L^2} \leq \tilde{C} \exp(-\tilde{c}n)$ while $\frac{d_n(\mathcal{H})_{L^2}}{d_n(\mathcal{H})_{L^2}} \sim n^{-1/2}$.

Similar results hold for manifolds resulting from more general hyperbolic equations.

A general result : if $F:V_1\to V_2$ is a L-Lipschitz mapping between Banach spaces, then an ϵ -net of $\mathcal{K}_1\subset V_1$ is mapped into an $L\epsilon$ -net of $\mathcal{K}_2:=F(\mathcal{K}_1)$ and therefore

$$\varepsilon_n(\mathcal{K}_2)_{V_2} \leq L\varepsilon_n(\mathcal{K}_1)_{V_1}, \quad n \geq 0.$$

This implies in particular that when V_2 is a Hilbert space

$$\sup_{n\geq 0} n^{s} \delta_{n,L}(\mathcal{K}_{1})_{V_{1}} < \infty \implies \sup_{n\geq 0} n^{s} \delta_{n,L}(\mathcal{K}_{2})_{V_{2}} < \infty.$$

Benchmark: develop concrete stable numerical methods that meet these rates

Stable width of solution manifolds

For the linear transport equation manifold $\mathcal{H}=\left\{\chi_{[a,a+1]}:a\in[a_{\min},a_{\max}]\right\}$ it is easily established that entropy numbers in L^p spaces have exponential decay

$$\varepsilon_n(\mathcal{H})_{L^p} \leq C \exp(-cn), \quad n \geq 0.$$

This implies in particular that $\delta_{n,L}(\mathcal{H})_{L^2} \leq \tilde{C} \exp(-\tilde{c}n)$ while $\frac{d_n(\mathcal{H})_{L^2}}{d_n(\mathcal{H})_{L^2}} \sim n^{-1/2}$.

Similar results hold for manifolds resulting from more general hyperbolic equations.

A general result : if $F:V_1\to V_2$ is a L-Lipschitz mapping between Banach spaces, then an ϵ -net of $\mathcal{K}_1\subset V_1$ is mapped into an $L\epsilon$ -net of $\mathcal{K}_2:=F(\mathcal{K}_1)$ and therefore

$$\varepsilon_n(\mathcal{K}_2)_{V_2} \leq L\varepsilon_n(\mathcal{K}_1)_{V_1}, \quad n \geq 0.$$

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Recent results in this direction

Consider a dictionnary $\mathcal D$ in a Hilbert space V, such that $\|\phi\|_V \leq 1$ for all $\phi \in \mathcal D$, and the model class

$$\mathcal{K} := \left\{ v = \sum c_j \varphi_j \ : \ \varphi_j \in \mathcal{D}, \ \sum |c_j| \leq 1 \right\}.$$

The OMP algorithm recursively produces

$$\label{eq:un} u_n = \sum_{j=1}^n c_j \phi_j = P_{V_n} u, \quad V_n = \mathrm{span}\{\phi_1, \dots, \phi_n\},$$

by selecting $\phi_n \in \mathcal{D}$ maximizing $\frac{\langle u - P_{V_{n-1}} u, \phi \rangle}{\|\phi\|_V}$ over $\phi \in \mathcal{D}$.

DeVore-Temlyakov (1998) : $u \in \mathcal{K} \implies ||u - u_n||_V \le n^{-1/2}$

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$$\mathcal{D} = \{ oldsymbol{arphi} = \mathcal{P}(oldsymbol{ heta}) \; : \; oldsymbol{ heta} \in \mathcal{M} \},$$

where \mathcal{M} is d-dimensional compact manifold and \mathcal{P} is \mathcal{C}^r . In this setting

$$u \in \mathcal{K} \implies \|u - u_n\|_V \lesssim n^{-s}, \quad s = \frac{1}{2} + \frac{r}{d} \quad \text{and} \quad \varepsilon_n(\mathcal{K})_V \lesssim n^{-s}.$$

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Sampling numbers (IBC - optimal recovery) measure the approximability of a class K from n point evaluations (critical quantity when such evaluations are costly).

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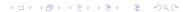
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THANKS

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THANKS!