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High-Dimensional Approximation

Part 1: Elements of approximation theory

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High dimensional problems

Many problems of computational science, statistics and probability require the approximation, integration or optimization of functions of many variables

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

- High dimensional PDEs (Boltzmann, Schrödinger, Black-Scholes...)
- Multiscale problems
- Parameter-dependent or stochastic equations
- Statistical learning (density estimation, classification, regression)
- Probabilistic modelling
- ...

Approximation

The goal of approximation is to replace a target function u by a simpler function (easy to evaluate and to operate with).

An approximation is searched in a set of functions X_n, where n is related to some complexity measure, typically the number of parameters.

Approximation

We distinguish

- linear approximation when X_n is a finite-dimensional linear space (polynomials, trigonometric polynomials, fixed knot splines...)

$$X_n = \{\sum_{i=1}^{n} a_i \varphi_i : a_i \in \mathbb{R}\}$$

  where the φ_i form a basis of X_n.

- nonlinear approximation when X_n is a nonlinear set (rational functions, free knot splines, n-term approximation, neural networks, tensor networks...), e.g.

$$X_n = \{\sum_{i=1}^{n} a_i \varphi_i : a_i \in \mathbb{R}, \varphi_i \in \mathcal{D}\}$$

  for n-term approximation from a dictionary of functions $\mathcal{D}$, or

$$X_n = \{g(a) : a \in \mathbb{R}^n\}$$

  with some given nonlinear map g from $\mathbb{R}^n$ to X.

Error of best approximation

For a given function u from a normed vector space X and a given subset X_n, the error of best approximation

$$e_n(u)_X := E(u, X_n)_X = \inf_{v \in X_n} \|u - v\|_X$$

quantifies the best we can expect from X_n.

Fundamental problems in approximation

For a sequence $(X_n)_{n\geq 1}$ of sets of growing complexity, called an approximation tool, we would like to address the following questions.

- (universality) Does $e_n(u)_X$ converge to 0 for all functions u in X ?
- (expressivity) For a certain class of functions in X, determine how fast $e_n(u)_X$ converges to 0, or determine the complexity $n = n(\epsilon, u)$ such that $e_n(u) \leq \epsilon$. Typically,

  $$e_n(u)_X \leq M\gamma(n)^{-1}$$

  where γ is a strictly increasing function (growth function), and

  $$n(\epsilon, u) \geq \gamma^{-1}(\epsilon/M)$$

- (approximation classes) Characterize the class of functions for which a certain convergence type is achieved, e.g.

  $$\mathcal{A}^\gamma(X, (X_n)_{n\geq 1}) = \left\{ u : \sup_{n\geq 1} \gamma(n) e_n(u)_X < +\infty \right\}$$

  for some growth function γ.

Fundamental problems in approximation

- (proximinality) Determine if for all $u \in X$, there exists an element of best approximation $u_n \in X_n$ such that

$$\|u - u_n\|_X = e_n(u)_X.$$

- (algorithm) Construct an approximation $u_n \in X_n$ such that

$$\|u - u_n\|_X \leq C e_n(u)_X$$

with C independent of n or $C(n)e_n(u) \to 0$ as $n \to \infty$.

Algorithms depend on the available information, e.g. given by linear functionals such as point evaluations (interpolation, discrete least-squares), or equations satisfied by the function (variational/Galerkin methods).

Optimal approximation for a model class

If we know that the function u belongs to some class of functions K, we would like to find an approximation tool X_n presenting a good performance, or even the optimal performance for that class.

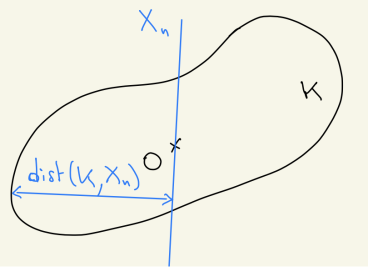
A fundamental problem is to quantify the best we can expect.

For that, we rely on different measures of complexity of K depending on the type of approximation (linear or nonlinear) and possibly on the properties of the approximation process (type of information, stability...)

Optimal linear approximation: Kolmogorov widths

For a compact subset K of a normed vector space X and a n-dimensional space X_n in X, we define the worst-case error

$$dist(K, X_n)_X = \sup_{u \in K} \inf_{v \in X_n} \|u - v\|_X$$

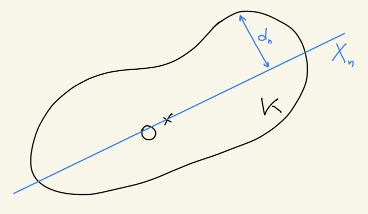


Optimal linear approximation: Kolmogorov widths

Then the Kolmogorov n-width of K is defined as

$$d_n(K)_X = \inf_{dim(X_n)=n} dist(K, X_n)_X$$

where the infimum is taken over all linear subspaces X_n of dimension n.



$d_n(K)_X$ measures how well the set K can be approximated (uniformly) by a n-dimensional space. It measures the ideal performance that we can expect from linear approximation methods.

Near to optimal spaces can be constructed by greedy algorithms (see in a next part).

Optimal linear approximation: weighted Kolmogorov widths

If K is equipped with a measure μ, a weighted Kolmogorov n-width is defined by

$$d_n^{(p,\mu)}(K)_X = \inf_{dim(X_n)=n} \left(\int_K E(u, X_n)_X^p d\mu(u) \right)^{1/p}.$$

If the measure is finite,

$$d_n^{(p,\mu)}(K)_X \leq \mu(K)^{1/p} d_n(K)_X.$$

For X a Hilbert space, $p = 2$ and μ the push-forward measure of a K-valued random variable $U \in L^2(\Omega; X)$, this is equivalent to

$$\inf_{dim(X_n)=n} \mathbb{E}(\|U - P_{X_n} U\|_X^2)^{1/2}$$

and an optimal space is given by Principal Component Analysis, that is a dominant eigenspace of the operator $v \mapsto \mathbb{E}((U, v)_X U)$ (see in a next part).

Optimal linear approximation: linear width

Another measure of complexity taking into account the approximation process is the linear width

$$a_n(K)_X = \inf_{A} \sup_{v \in K} \|v - Av\|_X$$

where the infimum is taken over all continuous linear maps $A : K \to X$ with rank at most n.

Equivalently,

$$a_n(K)_X = \inf_{g,a} \sup_{v \in K} \|v - g(a(v))\|_X$$

where both $a : K \to \mathbb{R}^n$ and $g : \mathbb{R}^n \to X$ are linear maps.

For a Hilbert space X,

$$a_n(K)_X = d_n(K)_X$$

For a general Banach space X,

$$d_n(K)_X \leq a_n(K)_X \leq \sqrt{n} d_n(K)_X$$

Optimal performance for linear approximation from point evaluations

By restricting the information to point evaluations, the performance is characterized by sampling numbers.

For deterministic information, the worst-case optimal performance for the approximation of functions in K is measured through the (linear) sampling number

$$\rho_n(K)_X = \inf_{\boldsymbol{x}} \inf_{A} \sup_{f \in K} \|f - A(f(x_1), \ldots, f(x_n))\|_X$$

where the infimum is taken over all linear maps A and points $\boldsymbol{x} = (x_1, \ldots, x_n) \in \mathcal{X}^n$, or equivalently

$$\rho_n(K)_X = \inf_{\boldsymbol{x}} \inf_{\varphi_1, \ldots, \varphi_n \in X} \sup_{f \in K} \|f - \sum_{i=1}^{n} f(x_i)\varphi_i\|_X$$

This quantifies the best we can expect from a linear algorithm using n samples for the approximation of functions in the class K.

Clearly,

$$\rho_n(K)_X \geq a_n(K)_X \geq d_n(K)_X$$

Optimal performance for linear approximation from point evaluations

For random information, the optimal performance can be measured in average mean squared error through the (linear) sampling number

$$\rho_n^{rand}(K)_X^2 = \inf_{\nu^n} \inf_{g} \sup_{f \in K} \mathbb{E}_{\boldsymbol{x} \sim \nu^n}(\|f - g(f(x_1), \dots, f(x_n))\|_X^2)$$

with an infimum taken over all measures ν^n on $\mathcal{X}^m$. Choosing for ν^n a dirac measure on an optimal deterministic set of points, we deduce that

$$d_n(K)_X \leq \rho_n(K)_X^{rand} \leq \rho_n(K)_X$$

The question is how far sampling numbers $\rho_n(K)_X$ or $\rho_n^{rand}(K)_X$ are from Kolmogorov widths $d_n(K)_X$, and how to generate optimal samples and algorithms in practice.

Optimal performance for linear approximation

A series of results have been recently obtained for L^2 approximation, comparing sampling numbers with Kolmogorov widths, e.g. [Cohen and Dolbeault 2021, Nagel, Schafer and Ullrich 2021, Temlyakov 2021, Dolbeault, Krieg and Ullrich 2022].

These results are based on constructive approaches for the approximation of functions in a given model class.

See in a next part.

Bounds of Kolmogorov widths $d_n(K)_X$

Upper bounds for $d_n(K)_X$ can be obtained by specific linear approximation methods. Proofs are sometimes constructive.

Lower bounds for $d_n(K)$ can be obtained using different techniques.

- Using diversity in K:

$$d_n(K)_X \geq d_n(S)_X$$

with S some subset of K whose Kolmogorov width can be bounded from below.

Example: if X is a Hilbert space and K contains a set of orthogonal vectors $S = \{u_1, \dots, u_m\}$ with norm $\|u_i\|_X = c_m$,

$$d_n(K)_X \geq d_n(S)_X = d_n(c_m B(\ell_1(\mathbb{R}^m)))_{\ell_2} = c_m \sqrt{1 - n/m}$$

where we used the fact that $d_n(S)_X$ is equal to the n-width of the balanced convex hull of S, which is isomorphic to $c_m B(\ell_1(\mathbb{R}^m))$, and a result of Stechkin (1954).

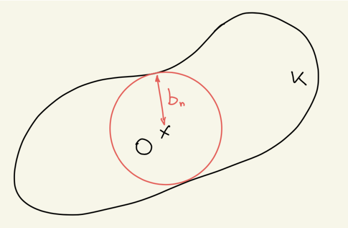
Bounds of Kolmogorov widths $d_n(K)_X$

- Using Bernstein width

$$b_n(K)_X = \sup_{\dim(X_{n+1})=n+1} \sup\{r : rB(X_{n+1}) \subset K\}$$

that is the largest $r > 0$ such that K contains the ball of radius r of some $(n+1)$-dimensional space

$$d_n(K)_X \geq b_n(K)_X$$

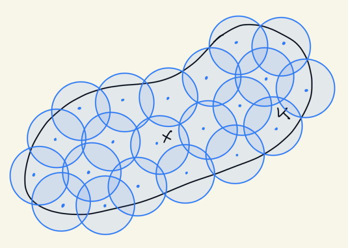


Bounds of Kolmogorov widths $d_n(K)_X$

- Using covering number $N_\epsilon(K)_X$ (minimal number of balls of radius ϵ for covering K) or entropy numbers

$$\epsilon_n(K)_X = \inf\{\epsilon : K \subset \bigcup_{i=1}^{2^n} B(u_i, \epsilon), u_i \in K\} = \inf\{\epsilon : \log_2(N_\epsilon(K)_X) \leq n\}$$

that is the smallest ϵ such that K can be covered by 2^n balls of radius ϵ. Any $u \in K$ can be encoded with n bits up to precision $\epsilon_n(K)$.



Carl's inequality: for all $s > 0$,

$$(n+1)^s \epsilon_n(K)_X \leq C_s \sup_{0 \leq m \leq n} (m+1)^s d_m(K)_X$$

Therefore, if $\epsilon_n(K)_X \gtrsim n^{-s}$, then $d_n(K)_X \lesssim n^{-r}$ can not hold with $r > s$.

Kolmogorov width of Sobolev balls

For $X = L^p(\mathcal{X})$, $\mathcal{X} = [0,1]^d$, $1 \leq p \leq \infty$, and K the unit ball of $W^{k,p}(\mathcal{X})$, it holds

$$d_n(K)_X \sim n^{-k/d}$$

and optimal performance is obtained e.g. by fixed knot splines (with degree adapted to the regularity).

We observe

- the curse of dimensionality : deterioration of the rate of approximation when d increases. Exponential growth with d of the complexity for reaching a given accuracy.
- the blessing of smoothness : improvement of the rate of approximation when k increases.

Kolmogorov width of mixed Sobolev balls

For $X = L^p(\mathcal{X})$, $\mathcal{X} = [0,1]^d$, $1 \leq p \leq \infty$, and K the unit ball of $MW^{k,p}(\mathcal{X})$ (Sobolev space with dominating mixed smoothness), that are functions u such that

$$\max_{|\alpha|_\infty \leq k} \|D^\alpha u\|_{L^p} \leq 1.$$

we have

$$d_n(K)_X \sim n^{-k} \log(n)^{k(d-1)}.$$

with optimal performance achieved by hyperbolic cross approximation (sparse expansion on tensor product of dilated splines) [Dung et al 2016].

Curse of dimensionality is milder but still present.

Optimal nonlinear approximation

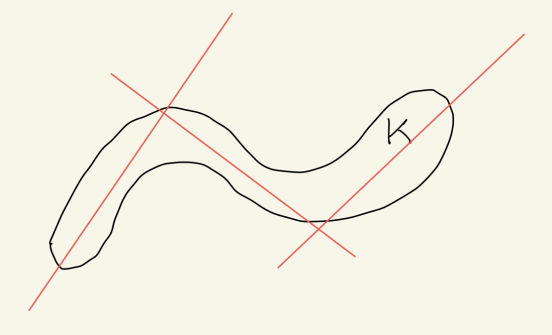
For evaluating the ideal performance of nonlinear methods for the approximation of functions from a class K, different notions of widths have been introduced.

Nonlinear Kolmogorov width

A measure of complexity closely related to n-term approximation and relevant for nonlinear model reduction is the nonlinear Kolmogorov width [Temlyakov 1998] or library width

$$d_n(K,N)_X = \inf_{\#\mathcal{L}_n = N} \sup_{u\in K} \inf_{V_n \in \mathcal{L}_n} E(u, V_n)_X$$

where the infimum is taken over all libraries $\mathcal{L}_n$ of N linear spaces of dimension n.



Choosing $N = N(n)$, this yields a width only depending on n. Interesting regimes are $N(n) = b^n$ or $N(n) = n^{\alpha n}$.

Nonlinear Kolmogorov width

It clearly holds

$$d_1(K, 2^n)_X \leq \epsilon_n(K)_X$$

Also, we have a Carl's type inequality: for all $r > 0$,

$$n^r \epsilon_n(K)_X \leq C(r, b) \max_{1 \leq k \leq n} k^r d_{k-1}(K, b^k)_X.$$

Therefore if for some $b > 0$, $d_{n-1}(K, b^n)_X \lesssim n^{-r}$, then $\epsilon_n(K)_X \lesssim n^{-r}$.

For unit balls K of Besov spaces $B^\alpha_q(L^\tau)$ compactly embedding in $L^p((0,1)^d)$, since $\epsilon_n(K) \gtrsim n^{-\alpha/d}$, we deduce that $d_n(K, b^n)_X \lesssim n^{-\beta}$ can not hold with $\beta > \alpha/d$.

Optimal nonlinear approximation: manifold approximation

Consider the approximation from a n-dimensional "manifold"

$$X_n = \{g(a) : a \in \mathbb{R}^n\}$$

parametrized by a nonlinear map $g : \mathbb{R}^n \to X$. We could consider the problem of finding the best manifold of dimension n for approximating functions from K:

$$\inf_g \sup_{u \in K} \inf_{a \in \mathbb{R}^n} \|u - g(a)\|_X := \eta_n$$

where the infimum is taken among all maps g from $\mathbb{R}^n$ to X.

For any compact set K, $\eta_n = 0$ for all $n \geq 1$. Indeed, K admits a countable dense subset $\{u_i\}_{i \in \mathbb{N}}$ (space-filling manifold). For $n = 1$, letting $g(a) = u_k$ for $a \in [k, k+1)$, we obtain $\eta_1 = 0$.

We can even provide a continuous parametrization, by considering a dense subset $\{u_i\}_{i \in \mathbb{Z}}$ and $g(a) = (a - k)u_{k+1} + (k + 1 - a)u_k$ for $a \in [k, k+1]$.

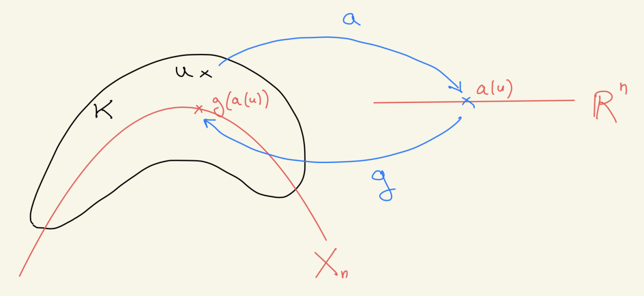
In general, the map which associates to $u \in K$ the coefficients $a(u)$ of its best approximation (if it exists) is not continuous, which makes the approximation process not reasonable.

Optimal nonlinear approximation: manifold width

The following definition of manifold width [DeVore, Howard, Michelli 1989] quantifies how well the set K can be approximated by n-dimensional nonlinear manifolds having continuous parametrization and a continuous parameter selection

$$\delta_n(K)_X = \inf_{g,a} \sup_{u \in K} \|u - g(a(u))\|_X$$

where the infimum is taken over all continuous functions a from K to $\mathbb{R}^n$ and all continuous functions g from $\mathbb{R}^n$ to K.



As for linear widths, the manifold width is lower bounded by the Bernstein width

$$\delta_n(K)_X \geq b_n(K)_X.$$

Manifold width of Sobolev balls

For $X = L^p(\mathcal{X})$, $\mathcal{X} = [0,1]^d$, and K the unit ball of Sobolev spaces $W^{s,q}$ or Besov spaces $B^s_q(L^\tau)$ which compactly embed in L^p

$$\delta_n(K)_X \sim n^{-s/d}$$

Rate $O(n^{-s/d})$ is achieved for a larger class of functions than for linear methods (functions with regularity measured in norms weaker than L^p) .

Optimal performance is achieved by free knot splines or best n-term approximation with a dictionary of tensor products of dilated splines.

Again, we observe the curse of dimensionality, which can not be avoided by such nonlinear methods.

Could extra regularity help ?

Consider $X = L^\infty(\mathcal{X})$ with $\mathcal{X} = [0,1]^d$ and

$$K = \{v \in C^\infty([0,1]^d) : \sup_\alpha \|D^\alpha u\|_{L^\infty} < \infty\},$$

It holds

$$K \subset B(W^{sd,\infty}) \quad \forall s > 0,$$

so that for all $s > 0$

$$d_n(K)_{L^\infty} \lesssim n^{-s}.$$

However,

$$\min\{n : d_n(K)_{L^\infty} \leq 1/2\} \geq c2^{d/2}.$$

The curse of dimensionality is still present.

Could extra regularity help ?

Consider the information based complexity measure of K

$$\delta_n^L(K)_{L^\infty} = \inf_{g,a} \sup_{u\in K} \|u - g(a(u))\|_{L^\infty} \leq a_n(K)_{L^\infty}$$

where the infimum is taken over all linear maps $a : K \to \mathbb{R}^n$ that extract n linear information $a_1(u), \dots a_n(u)$ from a function $u \in K$ (possibly selected adaptively) and over all nonlinear maps g.

It holds [Novak and Wozniakowski 2009]

$$\delta_n^L(K)_{L^\infty} = 1 \quad \text{for all } n = 0, 1, \dots, 2^{\lfloor d/2 \rfloor} - 1$$

or

$$\min\{n : \delta_n^L(K)_{L^\infty} < 1\} \geq 2^{\lfloor d/2 \rfloor}$$

Nonlinear methods can not help...

More assumptions of model classes K are needed...

Parameter dependent PDEs

Consider a parameter-dependent equation

$$\mathcal{P}(u(y); y) = 0, \quad u(y) \in X$$

with $y \in \mathcal{Y}$ some parameter.

The objective is to approximate the solution manifold (model reduction methods)

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

or to approximate explicitly the solution map $y \mapsto u(y)$.

As an example, consider the elliptic diffusion equation on a convex domain $D \subset \mathbb{R}^d$

$$-div(a(y)\nabla u(y)) = f$$

with $f \in H^{-1}$, $0 < \underline{a} \leq a(y) \leq \overline{a} < \infty$, and homogeneous Dirichlet boundary conditions.

The solutions

$$u(y) \in H_0^1 := X.$$

Parameter dependent PDEs

- Assuming $f \in L^2$ and $a(y)$ sufficiently smooth, we know that K is in some ball of $H^2(D)$, so that

$$d_n(K)_{H^1} \lesssim n^{-1/d}$$

with optimal performance achieved by splines (finite elements with uniform mesh).

- If $a(y) = a_0 + \sum_{i=1}^m a_i y_i$ with $(\|a_i\|_{L^\infty})_{i\geq 1} \in \ell_p$ for some $p > 1$, then

$$d_n(K)_{H^1} \leq C n^{-s}, \quad s = p^{-1} - 1$$

with constant C independent of d (no curse of dimensionality).

These rates are achieved by sparse polynomial expansions of $y \mapsto u(y)$, exploiting anisotropic analyticity of the solution map.

- More generally, letting $\mathcal{A} = \{a(y) : y \in \mathcal{Y}\}$, we have [Cohen and DeVore 2015]

$$\sup_{n\geq 1} n^s d_n(K)_{H^1} \lesssim \sup_{n\geq 1} n^r d_n(\mathcal{A})_{L^\infty}, \quad \forall s < r - 1.$$

- Optimal spaces X_n are data-dependent. Almost optimal spaces can be constructed using greedy algorithms (reduced basis methods) or sparse polynomial expansions.

- Similar results between nonlinear widths $\delta_n(K)_{H^1}$ and $\delta_n(\mathcal{A})_{L^q}$.

How to beat the curse of dimensionality ?

- No (reasonable) approximation tool is able to overcome the curse of dimensionality for standard regularity classes.

- The key is to make more assumptions on model classes of functions and to provide ad-hoc approximation tools .

- We would like flexible approximation tools that perform well for a wide range of applications (i.e. with sufficiently rich approximation classes)

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