The Curse of Dimension and a Universal Method For Numerical Integration

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Abstract. Many high dimensional problems are difficult to solve for any numerical method. This curse of dimension means that the computational cost must increase exponentially with the dimension of the problem. A high dimension, however, can be compensated by a high degree of smoothness. We study numerical integration and prove that such a compensation is possible by a recently invented method. The method is shown to be universal, i.e., simultaneously optimal up to logarithmic factors, on two different smoothness scales. The first scale is defined by isotropic smoothness conditions, while the second scale involves anisotropic smoothness and is related to partially separable functions.

1. Introduction

Several applications require the computation of high dimensional integrals. They are present, for example, in statistical mechanics, see [28] for an introduction. Another important example is the fast valuation of financial derivatives, see [16]. Some applications even require approximate values of path integrals, i.e., integrals over infinite dimensional spaces, see [30].

Limits of practical computability are often related to the high dimension of the problem. There is a "curse of dimension" which means that the minimal cost of computing an approximation grows exponentially in the dimension of the problem. Hence, many high dimensional numerical problems are practically impossible to solve. The curse of dimension was already observed by Bellman [3].

In addition to the number of variables, i.e., to the dimension, also the smoothness and the structure of the function is of importance. To a certain extent, a high dimension can be compensated by a high degree of smoothness and/or a favorable structure. As a rule, such a compensation cannot be achieved by means of classical methods. Hence we have to invent new methods.

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We want to expand the limits of practical computability by using, in an optimal way, the smoothness and the structure of the problem. We want to achieve this optimality even if the smoothness and the structure are unknown.

By smoothness we mean that the underlying functions have certain derivatives whose norms are not too large. By structure we mean certain geometrical properties, like convexity. Later we will discuss partially separable problems, another structural property. We will see that this property is strongly related to certain nonclassical smoothness classes of Nikolskii, Korobov, and Babenko.

It is a major goal of scientific computing to expand present limits of practical computability. To reach this goal, one should use the art and the techniques of computer science, such as parallel processing. First of all, however, it is very important to optimize the underlying algorithms with respect to their cost and accuracy. Optimal numerical methods can only be realized if the analytical model and the available information is fully used. This information-based view can exhibit the fundamental limits of practical computability. It is remarkable that these limits were already discussed by Kolmogorov, Bakhvalov, Nikolskii and Babenko, almost 40 years ago. Now these limits are systematically studied in the field of "information-based complexity", see [12,19,26,27,30].

In this paper we study numerical integration and further analyze a method that was introduced in [14]. In particular we prove that our method is almost optimal for each of the classical smoothness spaces C_d^r. The analogous result for the spaces F_d^r of functions with bounded mixed derivatives as well as many numerical examples are contained in our earlier paper. It is well known that classical methods, like product Gaussian rules, achieve the optimal order of convergence for all spaces C_d^r. However, these methods are useless if $d \geq 40$, say, while our method works with a relatively small number of knots even if the dimension d is large.

2. The Curse of Dimension

The curse of dimension occurs for many numerical problems. Assume that we want to compute a value $S(f)$ of a (linear or nonlinear) operator

$$S : X \to G$$

between two normed spaces. Often X is a space of functions f and we consider discretizations of S of the form

$$S_n(f) = \varphi(f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n)). \tag{1}$$

As the error criterion we often take the worst case error

$$e(S_n, X) = \sup_{f \in F} \|S(f) - S_n(f)\|$$

over the unit ball F of X. If S and S_n are linear then $e(S_n, X)$ is the operator norm of $S - S_n$. The total cost of computing $S_n(f)$ is at least n and often proportional to n. For simplicity we use here the number n of function evaluations as a measure for the cost. It should be stressed, however, that certain adaptive methods have a total cost that increases much faster than the number of function evaluations. The optimal error bounds

$$e_n(S, X) = \inf_{S_n} e(S_n, X)$$

indicate the best possible accuracy that can be achieved by any method with cost at most n.

Consider the standard smoothness classes

$$C_d^r = \{f : [-1,1]^d \to \mathbb{R} : \max_{|\alpha| \le r} \|f^{(\alpha)}\|_\infty < \infty\},$$

where $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$ is used to denote a partial derivative of order $|\alpha| = \alpha_1 + \ldots + \alpha_d$. For many problems, i.e, for many operators S, the optimal error bounds on the unit ball

$$F = \{f \in C_d^r : \max_{|\alpha| \le r} \|f^{(\alpha)}\|_\infty \le 1\}$$

in C_d^r satisfy

$$e_n(S, C_d^r) \asymp n^{-r/d}, \tag{2}$$

see, e.g., [12]. Here we use $\asymp$ to denote the weak equivalence of sequences, i.e., $v_n \asymp w_n$ iff $c_1 \le v_n/w_n \le c_2$ for sufficiently large n and positive constants c_i. The bound (2) holds, in particular, for the problem of numerical integration where

$$S(f) = \int_{[-1,1]^d} f(\mathbf{x})\, d\mathbf{x}.$$

Suppose that we want to construct an approximation S_n with error at most ε for a given positive and usually small or moderate ε. The cost n should be as small as possible. Then (2) yields

$$n \asymp \varepsilon^{-d/r}.$$

The curse of dimension means that the minimal cost n increases exponentially with the dimension d. Hence, the curse of dimension is present for many problems defined for the class C_d^r.

The proof of (2) consists of two parts. On the one hand we must prove a lower bound that is true for arbitrary methods of the form (1). On the other hand we must prove that there is a sequence $(S_n)_n$ of methods such that

$$e(S_n, C_d^r) \le c_{r,d} \cdot n^{-r/d} \tag{3}$$

for positive constants $c_{r,d}$. The upper bound (3) can be achieved by methods that use the function values from a regular grid. For the problem of numerical integration, for example, product formulas with the Gaussian method lead to the optimal order $n^{-r/d}$ for every r and every d.

Using the function values from a grid is a very classical idea that leads to practicable methods if d is small, say $d < 6$. Product rules cannot be applied, however, if d is large. Consider, for example, the case $d = 40$. If r is large, say $r = 80$ or even $r = \infty$, then the optimal order of convergence is not too bad, see (2). It is not clear, however, how to get practical methods since the smallest product method already needs 2^{40} points which is too large. Therefore the optimal order of product methods is only a theoretical result and we need new methods that realize (almost) the optimal order of convergence and can be used with a relatively small number of function values.

Known methods cannot fully use the existing smoothness if d is large, at least not for reasonable small values of n. Often Monte Carlo methods and/or number theoretic methods are used in high dimensions. Such methods can be applied for relatively small n but they can not fully use the smoothness properties of f, hence they cannot be used if a high accuracy is needed.

The error estimate (2) is a "negative" result if $d \gg r$. In this case the optimal error bounds $e_n(S, C_d^r)$ converge slowly and we should look for "smaller" classes $X \subset C_d^r$ that allow smaller errors and still contain many interesting functions.

3. Partially Separable Problems and Non-classical Function Spaces

Many high dimensional problems have a particular structure; they are partially separable. This means that f may depend on a huge number of variables but can be written as a sum of functions that only depend on few variables. A simple case would be

$$f(\mathbf{x}) = \sum_{1 \le i,j \le d} f_{i,j}(x_i, x_j) \tag{4}$$

where $\mathbf{x} = (x_1, \ldots, x_d)$. Here f is a sum of functions that only depend on two variables. At first glance it is not clear how we can use property (4) for numerical integration, if only function values of f can be computed.

Assume that $f_{i,j} \in C_2^2$ for each $f_{i,j}$ in the sum (4). Then $f \in C_d^2$, but in addition many higher order mixed derivatives exist. In particular, the derivative $f^{(\alpha)}$ with

$$\alpha = (1, \ldots, 1)$$

exists. Therefore f is in a class of functions with bounded mixed derivatives. Such classes were already studied by Nikolskii, Korobov, and Babenko in the sixties.

We consider the following scale of function spaces

$$F_d^r = \{f : [-1,1]^d \to \mathrm{I\!R} : \max_{\alpha \le r} \|f^{(\alpha)}\|_\infty < \infty\}$$

where $\alpha \le r$ means $\alpha_i \le r$ for every $i = 1, \ldots, d$. Let $f \in F_d^r$. Then $f^{(\alpha)}$ exists for

$$\alpha = (r, \ldots, r),$$

but the derivative $f^{(\alpha)}$ with

$$\alpha = (r+1, 0, \ldots, 0)$$

may not exist. Hence the class F_d^r is not isotropic. We stress that being of the form (4) with $f_{i,j} \in C_2^2$ is sufficient but not necessary for f to belong to the class F_d^1.

Because of their tight connection to partially separable functions we want to study the classes F_d^r, as well as the more traditional classes C_d^r. A given "smooth" function f usually is an element of several different classes F_d^r and/or C_d^r, the exact degree of smoothness often is not known to us. Moreover, different norms are used to define the unit balls in the scales F_d^r and C_d^r. The norms are nondecreasing in r while the error bounds are nonincreasing in r. Hence it is not obvious which choice of r in the condition $f \in F_d^r$ or $f \in C_d^r$ leads to the best error bound. This problem is sometimes called the fat F problem, see [31].

It is therefore important to have a "universal" method that is optimal (or almost optimal) for many different classes. Hence the following problem seems to be of great practical importance.

Problem: Construct optimal (or almost optimal) algorithms for C_d^r and F_d^r. In particular, find such algorithms

- simultaneously for all classes C_d^r and F_d^r;
- with good performance for a relatively small number n of knots.

Similar problems were studied in the univariate case by [4,17] and in the multivariate periodic case by [1,11,21,24,25,26]. We are interested in the general (i.e. nonperiodic) case and we have suggested a method in [14]. This method uses the full smoothness of the underlying function; it is not necessary to know the degree of smoothness in advance. Also the structural property "partially separable" is exploited optimally.

4. A Universal Method

We begin with the construction of Smolyak [23]. Special cases of this construction were invented independently for different applications and are known under different names, such as hyperbolic cross points methods, Boolean methods, discrete blending methods, and sparse grid methods. We give a partial list of references. Integration and approximation of functions is studied in [2,5,8,18]. See [6,7,9,33] for operator equations and [13] for global optimization. Problems for random functions are analyzed in [10,19,20,29]. Tractability of multidimensional problems is studied in [15,29,30,32].

We assume that for $d = 1$ a sequence of formulas

$$U^i(f) = \sum_{j=1}^{m_i} a_j^i \, f(x_j^i)$$

is given. In the case of numerical integration the a_j^i are just numbers. The method U^i uses m_i function values and we assume that U^{i+1} has smaller error than U^i and $m_{i+1} > m_i$. Define then, for $d > 1$, the tensor product formulas

$$(U^{i_1} \otimes \cdots \otimes U^{i_d})(f) = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_d=1}^{m_{i_d}} a_{j_1}^{i_1} \cdots a_{j_d}^{i_d} \, f(x_{j_1}^{i_1}, \ldots, x_{j_d}^{i_d}).$$

A tensor product formula clearly needs

$$m_{i_1} \cdot m_{i_2} \cdot \ldots \cdot m_{i_d}$$

function values, sampled on a regular grid. It is known that all tensor product formulas $S_n = U^{i_1} \otimes \cdots \otimes U^{i_d}$ lead to relatively large errors for the classes F_d^r, the optimal order of such methods is

$$e(S_n, F_d^r) \asymp e(S_n, C_d^r) \asymp n^{-r/d}.$$

The Smolyak formulas $A(q, d)$ are clever linear combinations of tensor product formulas such that:

- only tensor products with a relatively small number of knots are used;
- the linear combination is chosen in such a way that an interpolation property for $d = 1$ is preserved for $d > 1$.

The Smolyak formulas are defined by

$$A(q, d) = \sum_{q-d+1 \le |\mathbf{i}| \le q} (-1)^{q-|\mathbf{i}|} \cdot \binom{d-1}{q-|\mathbf{i}|} \cdot (U^{i_1} \otimes \cdots \otimes U^{i_d}),$$

where $q \ge d$.

The following method was suggested in [14]. Use, for $d > 1$, the Smolyak construction and start, for $d = 1$, with the classical Clenshaw-Curtis formula with

$$m_1 = 1 \quad \text{and} \quad m_i = 2^{i-1} + 1 \ \text{ for } \ i > 1.$$

The Clenshaw-Curtis formulas

$$U^i(f) = \sum_{j=1}^{m_i} a_j^i \, f(x_j^i)$$

use the knots

$$x_j^i = -\cos \frac{\pi(j-1)}{m_i - 1} \tag{5}$$

(and $x_1^1 = 0$). Hence we use nonequidistant knots. The weights a_j^i are defined in such a way that U^i is exact for all (univariate) polynomials of degree at most m_i. The resulting method has several remarkable properties, see [14]. In the next section we prove that it is almost optimal for the scale C_d^r; the analogous result for the scale F_d^r is already known.

5. Results

Let $A(q,d)$ denote the method from Section 4. First we cite an estimate on the number $n(q,d)$ of knots that are used by $A(q,d)$. We use $\approx$ to denote the strong equivalence of sequences, i.e., $v_n \approx w_n$ iff $\lim_{n\to\infty} v_n/w_n = 1$.

Lemma 1. *[10, Lemma 1]. For $k \to \infty$ and fixed d*

$$n(k+d,d) \approx \frac{1}{(d-1)! \cdot 2^{d-1}} \cdot 2^k\, k^{d-1}.$$

Smolyak's construction leads to cubature formulas with negative weights, even if positive weights are used in the univariate case. We show, however, that the weights are relatively small in absolute value. We use c_d and $c_{r,d}$ to denote different positive constants.

Lemma 2. *There exists a constant $c_d > 0$ such that*

$$\|A(q,d)\|_\infty \le c_d \cdot (\log(n(q,d)))^{d-1}.$$

Here $\|A(q,d)\|_\infty$ denotes the sum of the absolute values of the weights of $A(q,d)$.

Proof: Observe that

$$\#\{\mathbf{i} \in \mathbb{N}^d : \ |\mathbf{i}| = \ell\} = \binom{\ell-1}{d-1}.$$

Since the Clenshaw-Curtis formulas have positive weights, we conclude

$$\|A(q,d)\|_\infty \le c_d \cdot \sum_{\ell=q-d+1}^{q} \binom{\ell-1}{d-1} \le d \cdot \binom{q-1}{d-1} \le c_d \cdot q^{d-1}.$$

Due to Lemma 1,

$$\log n(q,d) \ge c_d \cdot q,$$

and the statement follows. ■

Now we present error bounds for our method $A(q,d)$ and the integration problem, i.e.,

$$S(f) = \int_{[-1,1]^d} f(\mathbf{x})\, d\mathbf{x}.$$

Theorem. *For $d, r \in \mathbb{N}$ there exists $c_{r,d} > 0$ such that*

$$e(A(q,d), F_d^r) \le c_{r,d} \cdot n^{-r} \cdot (\log n)^{(d-1)\cdot(r+1)}$$

and

$$e(A(q,d), C_d^r) \le c_{r,d} \cdot n^{-r/d} \cdot (\log n)^{(d-1)\cdot(r/d+1)},$$

where $n = n(q,d)$.

Proof: The error bound for the classes F_d^r is proven in [14]. In the sequel we analyze the error on C_d^r. Let $\mathbb{P}(\ell)$ be the space of all polynomials in one variable of degree at most ℓ. It turns out that $A(q,d)(f) = S(f)$ for all

$$f \in \sum_{|\mathbf{i}|=q} \mathbb{P}(m_{i_1}) \otimes \cdots \otimes \mathbb{P}(m_{i_d}),$$

see [14]. We conclude that $A(kd,d)$ is exact on

$$Z_k = \mathbb{P}(m_k) \otimes \cdots \otimes \mathbb{P}(m_k),$$

the space of polynomials of degree at most m_k in each variable. Therefore

$$e(A(kd,d), C_d^r) \le (2^d + \|A(kd,d)\|_\infty) \cdot \sup_{f \in F} \operatorname{dist}(f, Z_k), \tag{6}$$

where F denotes the unit ball in C_d^r and dist denotes the distance in the maximum norm. It is well known that

$$\sup_{f \in F} \operatorname{dist}(f, Z_k) \le c_{r,d} \cdot m_k^{-r}.$$

Applying Lemma 2 and $m_k \approx 2^{k-1}$ we obtain

$$e(A(kd,d), C_d^r) \le c_{r,d} \cdot (\log n(kd,d))^{d-1} \cdot 2^{-rk}.$$

Lemma 1 yields

$$\log n(kd,d) \approx kd + (d-1)\log k,$$

and therefore

$$e(A(kd,d), C_d^r) \le c_{r,d} \cdot (\log n(kd,d))^{(d-1)\cdot(r/d+1)} \cdot n(kd,d)^{-r/d}. \quad \blacksquare$$

Definition. *A sequence of quadrature formulas is called* universal *for a given scale of function spaces if it achieves, simultaneously for each member of the scale, the optimal order of convergence – up to logarithmic factors.*

Corollary. *The method $A(q,d)$ is universal for both the scales C_d^r and F_d^r.*

Proof: The upper bounds from the Theorem match the well known lower bounds for $e_n(S, C_d^r)$ and $e_n(S, F_d^r)$, respectively, up to logarithmic factors. This follows from the lower bound in (2) and $e_n(S, C_1^r) = e_n(S, F_1^r) \le e_n(S, F_d^r)$. $\blacksquare$

Remark 1. An analogous estimate to (6) shows that $A(q,d)(f)$ converges to the integral $S(f)$ whenever f is Hölder continuous for some exponent $\beta > 0$. More precisely,

$$e(A(q,d), X) \le c_{\beta,d} \cdot n^{-\beta/d} \cdot (\log n)^{(d-1)\cdot(\beta/d+1)}$$

on the respective unit ball. Nevertheless, in case of such low regularity equal weight formulas are likely to give better results.

On the other hand, consider classes X of analytic functions, where the distance

$$\sup_{f \in F} \operatorname{dist}(f, Z_k)$$

converges exponentially. Then we have exponential convergence of $e(A(q,d), X)$, again by the analogue to (6).

Remark 2. Our method is easily modified to work for weighted integrals

$$S(f) = \int_{[-1,1]^d} f(\mathbf{x}) \cdot \varrho(\mathbf{x})\, d\mathbf{x},$$

where

$$\varrho = \omega_1 \otimes \ldots \otimes \omega_d$$

is a tensor product. We only need to redefine the weights in the cubature formulas $A(q,d)$. In the univariate case we consider generalized Clenshaw-Curtis formulas

$$U^{i,\omega}(f) = \sum_{j=1}^{m_i} f(x_j^i) \cdot a_j^{i,\omega}$$

which use the knots x_j^i from (5) and are exact for all polynomials of degree less than m_i. Again we choose $m_1 = 1$ and $m_i = 2^{i-1}+1$ for $i > 1$ and apply Smolyak's construction to obtain cubature formulas $A(q,d)$. Observe that the set of knots is not changed.

It is known that

$$\lim_{i \to \infty} \sum_{j=1}^{m_i} |a_j^{i,\omega}| = \int_{-1}^{1} |\omega(x)|\, dx$$

if $\omega \in L_p([-1,1])$ for some $p > 1$, see [22]. In particular, the functionals $U^{i,\omega}$ are uniformly bounded on $C([-1,1])$. Assume that $\omega_1, \ldots, \omega_d \in L_p([-1,1])$ for some $p > 1$. As in the case $\varrho \equiv 1$ Lemma 2 and the error bound

$$e(A(q,d), C_d^r) \le c_{r,d} \cdot n^{-r/d} \cdot (\log n)^{(d-1)\cdot(r/d+1)}$$

follows. For the classes F_d^r the bound

$$e(A(q,d), F_d^r) \le c_{r,d} \cdot n^{-r} \cdot (\log n)^{(d-1)\cdot(r+1)}$$

is established in [14].

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