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Is there a curse of dimension for integration?

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INTRODUCTION

How does the cost of optimal methods increase with the dimension? We answer this question for integration of very smooth functions that are defined on the d-dimensional unit cube. For suitable classes of smooth functions the order of convergence of optimal methods does not depend on d. Nevertheless we prove exponential lower bounds for quadrature formulas with positive weights. Therefore the optimal order of convergence does not say much about the tractability or intractability of a problem.

This paper is about lower bounds, valid for arbitrary methods. The lower bounds are proved for the problem of numerical integration. Since numerical integration is part of the problem to solve a partial differential equation, these lower bounds can be applied to the (more difficult) problem of solving PDEs.

Let $\mathcal{F}_d$ be a class of functions defined on the unit cube $\Omega_d \subset \mathbf{R}^d$. We assume that $S_d : \mathcal{F}_d \to G_d$ is a sequence of operators which we want to approximate. For example $S_d(f) = u$ could be the solution of a linear PDE $Au = f$. To approximate S_d we use methods Q_n based on n function values,

$$Q_n(f) = \varphi(f(x_1), \ldots, f(x_n)), \tag{1}$$

where $\varphi : \mathbf{R}^d \to G_d$. The (worst case) error of Q_n is given by

$$e(Q_n) = \sup_{f \in \mathcal{F}_d} \|S_d(f) - Q_n(f)\|_{G_d},$$

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the nth minimal error by

$$e_n(\mathcal{F}_d) = \inf_{Q_n} e(Q_n).$$

The number $e_n(\mathcal{F}_d)$ is the error of the optimal method for the class $\mathcal{F}_d$, using at most n function values. The numbers

$$n(\varepsilon, d) = \min\{n \mid e_n(\mathcal{F}_d) \leq \varepsilon\}$$

are a measure for the complexity of computing the operators $S_d : \mathcal{F}_d \to G_d$.

In this paper we are mainly interested in lower bounds. We want to show that even for "simple" problems we have exponential lower bounds; hence there is an inherent "curse of dimension". Therefore we only consider the integration problem, where $G_d = \mathbf{R}$ and

$$S_d(f) = \int_{\Omega_d} f(x)\, dx.$$

Our classes $\mathcal{F}_d$ will be unit balls with respect to a norm. Then it is known that it is enough to study linear methods of the form

$$Q_n(f) = \sum_{i=1}^{n} c_i\, f(x_i) \tag{2}$$

with $c_i \in \mathbf{R}$ and $x_i \in \Omega_d$, since arbitrary nonlinear methods (1) cannot be better than linear methods (2), see [TWW88] or [Nov96]. For the classes $\mathcal{F}_d$ considered in this paper we have

$$e(Q_0) = e_0(\mathcal{F}_d) = 1, \tag{3}$$

where $Q_0(f) = 0$ is the trivial quadrature formula. Hence the problem is properly scaled for all d. We say that Q_n is positive if $c_i \geq 0$ for all $i = 1, \ldots, n$. Positive formulas are preferred due to their strong stability properties. Therefore we also define

$$e_n^+(\mathcal{F}_d) = \inf_{Q_n} e(Q_n),$$

where the infimum only runs through the set of positive quadrature formulas (2), and

$$n^+(\varepsilon, d) = \min\{n \mid e_n^+(\mathcal{F}_d) \leq \varepsilon\}.$$

The order of convergence of $e_n(\mathcal{F}_d)$ is known for many function classes $\mathcal{F}_d$. We often know that

$$e_n(\mathcal{F}_d) \asymp e_n^+(\mathcal{F}_d),$$

but we usually do not know whether $e_n(\mathcal{F}_d)$ and $e_n^+(\mathcal{F}_d)$ are equal. We only mention two specific results. Let $W_2^k([0,1]^d)$ be the classical Sobolev space with the norm

$$\|f\|_{W_2^k}^2 = \sum_{|\alpha| \leq k} \|D^\alpha f\|_{L_2}^2, \tag{4}$$

where $\alpha \in \mathbf{N}_0^d$ and $|\alpha| = \sum_{l=1}^d \alpha_l$, and let $BW_2^k([0,1]^d)$ be the unit ball of $W_2^k([0,1]^d)$. We assume the imbedding condition $2k > d$. It is well known that

$$e_n(BW_2^k([0,1]^d) \asymp e_n^+(BW_2^k([0,1]^d) \asymp n^{-k/d}.$$

Instead of BW_2^k, defined by the norm (4), we can define a set BH_2^k by the tensor product norm

$$\|f\|_{H_2^k}^2 = \sum_{\alpha_l \le k} \|D^\alpha f\|_{L_2}^2, \tag{5}$$

where the sum is over all $\alpha \in \mathbf{N}_0$ with $\alpha_l \le k$ for all l. We obtain a space $H_2^k([0,1]^d)$ of functions with bounded mixed derivatives and denote its unit ball by $BH_2^k([0,1]^d)$. It is known that

$$e_n(BH_2^k([0,1]^d) \asymp e_n^+(BH_2^k([0,1]^d) \asymp n^{-k} \cdot (\log n)^{(d-1)/2}. \tag{6}$$

In [NR96] we constructed quadrature formulas using *nonuniform sparse grids* based on the Chebyshev knots. These quadrature formulas have the following key properties, see also [NR97a] and [NR97b].

- *Simplicity.* The formulas can be easily computed for arbitrary dimensions d, also for weighted integrals with a weight ρ of tensor product form. We need $\mathcal{O}(n)$ arithmetic operations to compute the knots and weights of Q_n from suitable univariate quadrature formulas.
- *High Polynomial Exactness.* A small number of knots is sufficient to integrate all d-variate polynomials of a given degree exactly. We need

  $$n \approx 2^k/k! \cdot d^k$$

  knots for exactness of degree $2k+1$ if k is fixed and d is large. The well known lower bound is roughly $1/k! \cdot d^k$. Thus we have a polynomial dependence on the dimension d, and the exponent k is best possible.
- *Universality.* Small errors are guaranteed for many different smoothness classes. If f has bounded derivatives up to order k then

  $$|I_d(f) - Q_n(f)| = \mathcal{O}\big(n^{-k/d} \cdot (\log n)^{(d-1)(k/d+1)}\big). \tag{7}$$

  If f has a bounded mixed derivative $f^{(k,\dots,k)}$ then

  $$|I_d(f) - Q_n(f)| = \mathcal{O}\big(n^{-k} \cdot (\log n)^{(d-1)(k+1)}\big). \tag{8}$$

  These two estimates are optimal – up to logarithmic factors – in both smoothness scales. The bounds (7) and (8) hold for all $k \in \mathbf{N}$, hence the method is not only almost optimal for a specific class of integrands but universal, i.e., it is almost optimal for many different function classes.

Sparse grids with equidistant sets of knots were often studied in the literature. Some authors mainly discuss periodic functions and then equidistant knots are quite adequate, see [Tem93] and [CNR98]. We prefer to study the general (nonperiodic) case and then it is much better, already for $d=1$, to use nonequidistant knots, such as the Chebyshev knots. These knots, or modifications of these knots, were also used by [Coo98], [FH96], [GG98], and [NRSS97]. In [NRS98] we discuss related quadrature formulas for the Wiener measure, see [Ste99] for the proof of polynomial error bounds. For the problem of *interpolation* or *optimal recovery*, see [BNR98], [Spr97a], and [Spr97b].

The order of $e_n(BH_2^k([0,1]^d)$ is between n^{-k} and $n^{-k+\delta}$, for any $\delta > 0$, independently of d. Hence we may say that the *order of convergence* does *not* depend on d. It is tempting to say that the complexity of the problem does not depend on d, there is no curse of dimension. We will show in the following that such a conclusion would be wrong.

Consider the following problem. Assume that $k \in \mathbf{N}$ is fixed and consider

$$n^+(\varepsilon, d) = \inf\{n \mid e_n^+(BH_2^k([0,1]^d) \le \varepsilon\}.$$

The problem is to verify whether $n^+(\varepsilon, d)$ depends polynomially on d and ε^{-1}. If so then the problem is *tractable*, if not then it is *intractable*. Observe that the known order (6), with unknown constants that depend on d, does not say anything about tractability. We proved in [Nov98] that the problem is intractable since

$$e_n^+(BH_2^k([0,1]^d)^2 \ge 1 - n \cdot c_k^d,$$

where $c_k < 1$ does not depend on d. It is still open whether such a lower bound also holds for the e_n, i.e., for arbitrary quadrature formulas.

We now consider "very smooth" functions. We use the norm

$$\|f\|_{F_d}^2 = \sum_{\alpha \in \mathbf{N}_0^d} \|D^\alpha f\|_{L_2}^2 \tag{9}$$

and define

$$F_d = \{f : \Omega \to \mathbf{R} \mid \|f\|_{F_d} \le 1\}.$$

Observe that

$$F_d \subset \bigcap_{k=1}^{\infty} BH_2^k([0,1]^d)$$

which yields

$$e_n^+(F_d) \le c_{d,k} \cdot n^{-k}$$

for *all* $d, k \in \mathbf{N}$, where $c_{d,k} > 0$ depends on d and k. Moreover we have $e_1^+(F_d) = 1$ for all d, so the problem is properly scaled and the order of convergence is very high for all d.

Nevertheless we will prove the exponential (in d) lower bound

$$e_n^+(F_d)^2 \ge 1 - n \cdot c^d,$$

where $c = 0.995$, for positive quadrature formulas. For the proof it is convenient to consider even smaller classes BV_d of functions. The BV_d contain polynomials of degree at most two in each variable. For any fixed $\varepsilon < 1$ we need a number n of sample points which increases exponentially with the dimension. We do not know whether arbitrary quadrature formulas for the class F_d are better than positive quadrature formulas.

We finish this section by a bibliographic remark. Explicit *upper* bounds (without unknown constants) were recently obtained by [WW95] and [WW98]. The paper of [SW98] contains *upper and lower* bounds for certain tensor product Hilbert spaces and for quasi-Monte Carlo methods, i.e., for formulas with equal weights $c_i = 1/n$. Some lower bounds can be generalized to the class of positive quadrature formulas, see [Nov98] and [Woź98]. General results about tractability of linear problems can be found in [Woź94a], [Woź94b], and [NSW97]. For related results see also [SW97] and [HW99].

OPTIMAL ERROR BOUNDS AND OTHER EXTREMAL PROBLEMS

We begin with the definition of the classes V_d of functions on Ω_d. Here Ω_d is the unit cube in $\mathbf{R}^d$ which we define, for convenience, in a shifted way through $\Omega_d = [-1/2, 1/2]^d$. The space V_1 is generated by $f_1 = 1$, $f_2(x) = x$, and $f_3(x) = x^2$. These functions are not orthogonal, with respect to the usual Sobolev-Hilbert norms

$$\|f\|^2_{W_2^k} = \sum_{j=0}^{k} \|D^j f\|^2_{L_2}, \tag{10}$$

and hence we prefer the functions $e_1 = 1$, $e_2(x) = x$, and $e_3(x) = x^2 - 1/12$. The e_i are orthogonal for each norm (10). We obtain $\|e_1\|_{W_2^k} = 1$ for all k,

$$\|e_2\|_{W_2^k} = (1 + 1/12)^{1/2}$$

for all $k \geq 1$, and

$$\|e_3\|_{W_2^k} = (4 + 1/3 + 1/180)^{1/2}$$

for all $k \geq 2$. We define a scalar product on V_1 by $(e_i, e_j) = 0$ for $i \neq j$ and

$$(e_1, e_1) = 1, \quad (e_2, e_2) = 13/12, \quad \text{and} \quad (e_3, e_3) = (4 + 1/3 + 1/180).$$

We denote by BV_1 the unit ball of V_1 with respect to this norm. The norm on V_1 coincides with the k-norm (10) for each $k \geq 2$ and also with the norm (9).

For $d > 1$, we define V_d as the tensor product $V_d = V_1 \otimes \ldots \otimes V_1$ (d times). The dimension of V_d is 3^d. On the space V_d we define the tensor product (cross-) norm by

$$(f_1 \otimes \ldots \otimes f_d,\, g_1 \otimes \ldots \otimes g_d) := \prod_{m=1}^{d} (f_m, g_m). \tag{11}$$

Let BV_d denote the unit ball of V_d. The norm defined by (11) is the same as (5), for each $k \geq 2$, and is the same as (9). Hence we obtain $BV_d \subset F_d$ and $e_n^+(BV_d) \leq e_n^+(F_d)$. Observe that

$$I_d(f) = (f, 1) \qquad \text{and} \qquad \|1\| = 1,$$

for all $d \in \mathbf{N}$. It follows that $e(Q_0, BV_d) = e_0(BV_d) = 1$, see (3).

A Dirac functional $f \mapsto f(x)$ can be written in the form

$$f(x) = (\delta_x, f)$$

for all $f \in V_d$ since we have a kernel reproducing Hilbert space. Here δ_x is a suitable element of V_d which is a tensor product of the respective δ_{x^m}, where $x = (x^1, \ldots, x^d)$ and $\delta_{x^m} \in V_1$. To find the

$$\delta_x = \sum_{j=1}^{3} c_j(x)\, e_j$$

in the case $d = 1$, we have to solve the linear system $e_i(x) = c_i(x)\,(e_i, e_i)$, for $i = 1, 2, 3$, and get

$$c_1(x) = 1, \qquad c_2(x) = \frac{12x}{13}, \qquad c_3(x) = \frac{x^2 - 1/12}{4 + 1/3 + 1/180}.$$

Therefore we obtain the following lemma.

Lemma 1 *The kernel k_1 of V_1 is given by*

$$k_1(x,y) = (\delta_x, \delta_y) = 1 + \frac{12xy}{13} + \frac{(x^2-1/12)(y^2-1/12)}{4+1/3+1/180}.$$

For $d>1$ the kernel is given by

$$k_d(x,y) = (\delta_x, \delta_y) = \prod_{m=1}^{d} k_1(x^m, y^m),$$

where $x = (x^1, \ldots, x^d)$.

Later we need the values

$$k_{\min} = \inf_{x,y} k_1(x,y) \approx 0.94 \qquad \text{and} \qquad k_{\max} = \inf_{x} k_1(x,x) \approx 1.005.$$

For our approach it is important that the kernel is positive, $k_1(x,y) \geq 0$. It is easy to check that

$$e(Q_n, BV_d) = \left\| 1 - \sum_{i=1}^{n} c_i\, \delta_{x_i} \right\|$$

for Q_n of the form (2). The optimal error bounds $e_n(BV_d)$ for quadrature formulas are related to the solution of the following extremal problem for polynomials. For given points $x_i \in \Omega_d$ find

$$f \in V_d \quad \text{with} \quad f(x_1) = \ldots = f(x_n) = 1 \quad \text{and} \quad \|f\| \to \min!$$

We define the numbers

$$g(n,d) = \sup_{x_1,\ldots,x_n} \inf\{\|f\|^2 \,:\, f \in V_d,\ f(x_1) = \ldots = f(x_n) = 1\}.$$

Then one can prove that $g(n,d) + e_n(BV_d) = 1$, the proof is similar as in [Nov98], where a different kernel and periodic functions were studied. It follows that for $d, n \in \mathbf{N}$ and $\Phi > 0$ the following statements are equivalent:

(a) $e_n^+(BV_d)^2 \geq 1 - \Phi$;

(b) Any linear system of the form

$$\sum_{i=1}^{m} c_i\, k_d(x_i, x_j) = 1, \tag{12}$$

$j = 1, \ldots, m$, with $m \leq n$ and a solution that satisfies $c_i \geq 0$ for all i fulfills $\sum_{i=1}^{m} c_i \leq \Phi$.

Consider the linear system (12) for $c_i \geq 0$. The diagonal elements are at least $k_{\max}^d$ and the off-diagonal elements are at least $k_{\min}^d$. Summing up all the equations we get

$$m \;=\; \sum_{i,j=1}^{m} c_i\, k_d(x_i, x_j) \geq \sum_{i=1}^{m} c_i \left(k_{\max}^d + (m-1) k_{\min}^d\right).$$

This yields

$$\sum_{i=1}^{m} c_i \le \frac{m}{k_{\max}^d + (m-1)k_{\min}^d} \le \frac{n}{k_{\max}^d + (n-1)k_{\min}^d}.$$

Hence we obtain the following lower bound.

Theorem 1 *Let $d, n \in \mathbf{N}$. Then*

$$e_n^+(BV_d)^2 \ge 1 - n \cdot \left(k_{\max}^d + (n-1)k_{\min}^d\right)^{-1}.$$

We end this paper with a remark. We showed that high dimensional integration is intractable for positive quadrature formulas, even if the functions are very smooth. If weighted norms are considered, however, then certain high dimensional integrals can be computed efficiently, see [SW98] and [Nov98].

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