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A Tractability Result for the Clenshaw Curtis Smolyak Algorithm

A. Hinrichs, E. Novak, M. Ullrich

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A Tractability Result for the Clenshaw Curtis Smolyak Algorithm

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Abstract

We consider the problem of integration of d -variate analytic functions defined on the unit cube with directional derivatives of all orders bounded by 1. We prove that the Clenshaw Curtis Smolyak algorithm leads to weak tractability of the problem. This seems to be the first positive tractability result for the Smolyak algorithm for a normalized and unweighted problem. The space of integrands is not a tensor product space and therefore we have to develop a different proof technique. We use the polynomial exactness of the algorithm as well as an explicit bound on the operator norm of the algorithm.

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1 Introduction and Result

We prove that the Clenshaw Curtis Smolyak algorithm is weakly tractable for a class of analytic functions. To explain this result, we say a few words about this algorithm, about recent tractability results, and about our proof technique.

1.1 The CCS algorithm

We want to compute

$$S_d(f) = \int_{[0,1]^d} f(x) dx$$

and use the Smolyak algorithm [27] in combination with the Clenshaw Curtis algorithm as in Novak, Ritter [16, 17, 18], see also Gerstner, Griebel [9] and Petras [23]. We describe the resulting CCS algorithm.

For $f: [0, 1] \rightarrow \mathbb{R}$ define the sequence of (one-dimensional) quadrature rules

$$U^\ell(f) = \sum_{j=1}^{m_\ell} a_j^\ell f(x_j^\ell), \quad \ell \in \mathbb{N}, \quad (1)$$

with

$$m_\ell = \begin{cases} 1, & \ell = 1 \\ 2^{\ell-1} + 1, & \ell \geq 2, \end{cases}$$

nodes

$$x_j^\ell = \frac{1}{2} \left(1 - \cos \left(\pi \frac{j-1}{m_\ell-1} \right) \right), \quad j = 1, \dots, m_\ell$$

and weights

$$a_j^\ell = \begin{cases} \frac{1}{2m_\ell(m_\ell-2)}, & j = 1, m_\ell \\ \frac{1}{m_\ell-1} \left(1 - \frac{\cos(j-1)\pi}{(m_\ell-1)^2-1} - 2 \sum_{k=1}^{\frac{m_\ell-3}{2}} \frac{\cos \frac{2k(j-1)\pi}{m_\ell-1}}{4k^2-1} \right), & j = 2, \dots, m_\ell-1 \end{cases} \quad (2)$$

for $\ell > 1$. For $\ell = 1$ there is only one node $x_1^1 = 1/2$ with weight $a_1^1 = 1$. These rules are called Clenshaw-Curtis (CC) quadrature rules. It is well known that the CC-rules are positive rules, that is $a_j^\ell > 0$ for all j and ℓ , see [4].

Observe that the nodes of the U^ℓ are nested, since

$$x_{2j-1}^{\ell+1} = x_j^\ell \quad \text{for } j = 1, 2, \dots, m_\ell.$$

Additionally, we define

$$\Delta^1 = U^1 \quad \text{and} \quad \Delta^\ell = U^\ell - U^{\ell-1}, \quad \ell \geq 2. \quad (3)$$

Note that, for $f: [0, 1] \rightarrow \mathbb{R}$,

$$\Delta^\ell(f) = \sum_{j=1}^{m_\ell} b_j^\ell f(x_j^\ell), \quad \ell \in \mathbb{N},$$

with

$$b_j^\ell = \begin{cases} a_j^\ell & \text{for even } j \\ a_j^\ell - a_{\frac{j+1}{2}}^{\ell-1} & \text{for odd } j. \end{cases}$$

These weights, except for $\ell = 1$, sum up to zero.

Then the Smolyak algorithm (based on the CC rule U^ℓ) is defined by

$$A(q, d) = \sum_{i \in \mathbb{N}_0^d: |i| \leq q-d} \Delta^{i_1+1} \otimes \dots \otimes \Delta^{i_d+1}.$$

Here, the d -fold tensor product of the functionals Δ^ℓ is given by

$$(\Delta^{\ell_1} \otimes \dots \otimes \Delta^{\ell_d})(f) = \sum_{j_1=1}^{m_{\ell_1}} \dots \sum_{j_d=1}^{m_{\ell_d}} b_{j_1}^{\ell_1} \cdot \dots \cdot b_{j_d}^{\ell_d} f(x_{j_1}^{\ell_1}, \dots, x_{j_d}^{\ell_d})$$

for $f: [0, 1]^d \rightarrow \mathbb{R}$. Note that we can write this CCS algorithm $A(q, d)$, for $q = d + k$, as

$$A(d + k, d) = \sum_{\ell=1}^{k+1} A(d + k - \ell, d - 1) \otimes \Delta^\ell.$$

The Smolyak algorithm can also be written as

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

see Wasilkowski and Woźniakowski [30, Lemma 1]. Clearly $A(q, d)$ is a linear functional, and $A(q, d)(f)$ depends on f only through function values at a finite number of points. To describe these points let

$$X^i = \{x_1^i, \dots, x_{m_i}^i\} \subset [0, 1]$$

denote the set of nodes of U^i . The tensor product algorithm $U^{i_1} \otimes \dots \otimes U^{i_d}$ is based on the grid $X^{i_1} \times \dots \times X^{i_d}$, and therefore $A(q, d)(f)$ depends (at most) on the values of f at points in the union

$$H(q, d) = \bigcup_{q-d+1 \leq |i| \leq q} (X^{i_1} \times \dots \times X^{i_d}) \subset [0, 1]^d$$

of grids. Nested sets $X^i \subset X^{i+1}$ yield $H(q, d) \subset H(q+1, d)$ and

$$H(q, d) = \bigcup_{|i|=q} (X^{i_1} \times \dots \times X^{i_d}).$$

Therefore nested sets seem to be the most economical choice. The points $x \in H(q, d)$ are called hyperbolic cross points and $H(q, d)$ is also called a sparse grid.

In what follows we will bound the number of function values that are sufficient for the CCS algorithm to achieve a certain error. For this we define

$$N_d(k) := |H(d+k, d)|$$

as the number of points used by $A(d+k, d)$.

1.2 Some known properties of the CCS algorithm

Error bounds for the Smolyak algorithm were proved by Smolyak [27], Wasilkowski and Woźniakowski [30] and many others, see also [22]. In this paper we always consider the worst case error with respect to the unit ball for some norm, and therefore properties of various norms are very relevant.

Most of the known error bounds are for tensor product spaces, i.e., one takes norms with

$$\|f_1 \otimes f_2 \otimes \dots \otimes f_d\| = \prod_{i=1}^d \|f_i\|, \quad (4)$$

where

$$(f_1 \otimes f_2 \otimes \dots \otimes f_d)(x) = \prod_{i=1}^d f_i(x_i).$$

We stress that in this paper we do *not* use tensor product norms since we use the norm

$$\sup_{k \in \mathbb{N}_0} \sup_{\theta \in S^{d-1}} \|D_\theta^k f\|_\infty, \quad (5)$$

where $D_\theta f$ denotes the directional derivative of f in direction θ . Therefore we cannot use the property (4) and error bounds based on it. We want to illustrate this a bit further using

the functions $f_1(x) = x$ and $f_2(x) = x^2$, where $f_i : [0, 1] \rightarrow \mathbb{R}$. Clearly all partial derivatives of $f_1 \otimes f_1 \otimes \cdots \otimes f_1$ are bounded by 1. Some directional derivatives are larger than 1 and hence, for the norm (5),

$$\|f_1 \otimes f_1\| > \|f_1\| \cdot \|f_1\|.$$

This property makes the unit ball with respect to the norm (5) *smaller* than the unit ball of a tensor product space.

Consider now $C^r([0, 1]^d)$ with the standard norm

$$\|f\| = \max_{|\alpha| \leq r} \|D^\alpha f\|_\infty, \quad (6)$$

where $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$ is used to denote a partial derivative of order $|\alpha| = \alpha_1 + \cdots + \alpha_d$. Then, for $r = 1$,

$$2 = \|f_2 \otimes f_2\| < \|f_2\| \cdot \|f_2\| = 4.$$

This property makes the unit balls of $C^k([0, 1]^d)$ *larger* than the unit balls of tensor product spaces. We present a result from [17] for the CCS algorithm for the order of convergence and the standard norm (6), hence the unit ball is

$$C_d^r = \{f : [0, 1]^d \rightarrow \mathbb{R} \mid \max_{|\alpha| \leq r} \|f^{(\alpha)}\|_\infty \leq 1\}.$$

Proposition 1. For $d, r \in \mathbb{N}$ there exists $c_{r,d} > 0$ such that

$$e(A(q, d), C_d^r) = \sup_{f \in C_d^r} |A(q, d)(f) - S_d(f)| \leq c_{r,d} \cdot N^{-r/d} \cdot (\log N)^{(d-1) \cdot (r/d+1)}, \quad (7)$$

where $N = N_d(q - d)$ is the number of function values used by the CCS algorithm.

We describe the proof since in this paper we use a similar technique, but with a different emphasis. Observe that Proposition 1 contains unknown constants $c_{r,d}$ and hence the error bound makes sense only for given r and d and very large N or small error ε . For the proof we need three facts.

First we need an estimate of the number $N_d(k)$ of knots that are used by $A(d + k, d)$. We use \approx to denote the strong equivalence of sequences, i.e., $v_n \approx w_n$ iff $\lim_{n \rightarrow \infty} v_n/w_n = 1$. Then, for $k \rightarrow \infty$ and fixed d ,

$$N_d(k) \approx \frac{1}{(d-1)! \cdot 2^{d-1}} \cdot 2^k k^{d-1}, \quad (8)$$

see Müller-Gronbach [14, Lemma 1].

Smolyak's construction leads to cubature formulas with negative weights, even if positive weights are used in the univariate case. However, the weights are relatively small in absolute value. Hence, secondly, we need a bound for $\|A(q, d)\|$, where $\|A(q, d)\|$ denotes the sum of the absolute values of the weights of $A(q, d)$. We use c_d and $c_{r,d}$ to denote different positive constants depending on d or on r and d , respectively. There exists a constant $c_d > 0$ such that

$$\|A(d+k, d)\| \leq c_d \cdot \left(\log(N_d(k)) \right)^{d-1}. \quad (9)$$

For a proof observe that

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

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

$$\|A(d+k, d)\| \leq c_d \cdot \sum_{\ell=k+1}^{d+k} \binom{\ell-1}{d-1} \leq c_d \cdot \binom{d+k-1}{d-1} \leq c_d \cdot (d+k)^{d-1}, \quad (10)$$

where we can take $c_d = 2^d$. Then (9) follows from

$$\log N_d(k) \geq c_d \cdot (d+k).$$

The third fact that we need is that $A(d+k, d)$ is exact for all polynomials of total degree at most $2k+1$, see [16, 18]. \square

We add in passing that the estimates (8), (9) and (10) are not suitable for tractability studies. In particular we cannot use estimates that contain unknown or exponentially large constants c_d .

1.3 The curse of dimensionality

We study multivariate integration for different classes F_d of smooth functions $f: [0, 1]^d \rightarrow \mathbb{R}$. Our emphasis is on large values of $d \in \mathbb{N}$. We want to approximate

$$S_d(f) = \int_{D_d} f(x) dx \quad \text{for } f \in F_d \quad (11)$$

up to some error $\varepsilon > 0$.

We consider (deterministic) algorithms that use only function values, and classes F_d of functions bounded in absolute value by 1 and containing all constant functions $f(x) \equiv c$

with $|c| \leq 1$. An algorithm that uses no function value at all must be a constant, $A_0(f) \equiv b$, and its error is at least

$$\max_{f \in F_d} |S_d(f)| = 1.$$

We call this the initial error of the problem, it does not depend on d . Hence multivariate integration is well scaled and that is why we consider $\varepsilon < 1$.

Let $n(\varepsilon, F_d)$ denote the minimal number of function values needed for this task in the worst case setting. By the *curse of dimensionality* we mean that $n(\varepsilon, F_d)$ is exponentially large in d . That is, there are positive numbers c , ε_0 and γ such that

$$n(\varepsilon, F_d) \geq c(1 + \gamma)^d \quad \text{for all } \varepsilon \leq \varepsilon_0 \quad \text{and infinitely many } d \in \mathbb{N}. \quad (12)$$

For many natural classes F_d the bound in (12) will hold for all $d \in \mathbb{N}$. There are many classes F_d for which the curse of dimensionality has been proved, see [20, 22] for such examples.

The classes C_d^r were already studied in 1959 by Bakhvalov [2], see also [15]. He proved that there are two positive numbers $c_{r,d}$ and $\tilde{c}_{r,d}$ such that

$$c_{r,d} \varepsilon^{-d/r} \leq n(\varepsilon, C_d^r) \leq \tilde{c}_{r,d} \varepsilon^{-d/r} \quad \text{for all } d \in \mathbb{N} \text{ and } \varepsilon \in (0, 1). \quad (13)$$

This means that for a fixed d and for ε tending to zero, we know that $n(\varepsilon, C_d^r)$ is of order $\varepsilon^{-d/r}$ and the exponent of ε^{-1} grows linearly in d . If we compare this with Proposition 1 we may say that the CCS algorithm is “almost optimal” for each class C_d^r . In this sense the algorithm is “universal”.

Bakhvalov’s result does not allow us to conclude whether the curse of dimensionality holds for the classes C_d^r . In fact, if we reverse the roles of d and ε , and consider a fixed ε and d tending to infinity, the bound (13) on $n(\varepsilon, C_d^r)$ is useless. The curse of dimensionality for the classes C_d^r was only recently proved in Hinrichs, Novak, Ullrich and Woźniakowski [11].

Proposition 2. The curse of dimensionality holds for the classes C_d^r with the *super-exponential* lower bound

$$n(\varepsilon, C_d^r) \geq c_r (1 - \varepsilon) d^{d/(2r+3)}$$

for all $d \in \mathbb{N}$ and $\varepsilon \in (0, 1)$, where $c_r \in (0, 1]$ depends only on r .

One may say that the classes C_d^r are too large and therefore we obtain the curse of dimensionality. Therefore it is natural to study smaller classes such as the unit balls F_d with respect to the norm (5). In Hinrichs, Novak, Ullrich and Woźniakowski [12] we prove

Proposition 3. The curse of dimensionality does not hold for the classes F_d since the problem is weakly tractable, i.e.,

$$\lim_{d+\varepsilon^{-1} \rightarrow \infty} \frac{\log(n(\varepsilon, F_d))}{d + \varepsilon^{-1}} = 0.$$

This means that, for a fixed ε , the complexity of integration is sub-exponential in the dimension. Unfortunately, the proof of Proposition 3 in [12] is rather theoretical, we use a very unstable algorithm which is based on the approximation of high derivatives by function values via finite differences, see also Vybíral [29]. This algorithm could not be implemented because of huge rounding errors. The aim of this paper is to give a much more constructive proof of Proposition 3 by means of the CCS algorithm, see Theorem 4.

1.4 Main result

Let

$$F_d = \left\{ f \in C^\infty([0, 1]^d) \mid \sup_{k \in \mathbb{N}_0} \sup_{\theta \in S^{d-1}} \|D_\theta^k f\|_\infty \leq 1 \right\}, \quad (14)$$

where $D_\theta f$ denotes the directional derivative of f in direction θ .

Theorem 4. For each $d \in \mathbb{N}$ and $\varepsilon \in (0, 1]$ define

$$k_{\varepsilon, d} := \left\lceil \max \left\{ 3 d^{2/3}, \ln(1/\varepsilon) \right\} \right\rceil.$$

Then,

$$e(k_{\varepsilon, d}, d) := \sup_{f \in F_d} |A(d + k_{\varepsilon, d})(f) - S_d(f)| \leq \varepsilon$$

and the number of function values $N_d(k_{\varepsilon, d})$ used by the CCS algorithm $A(d + k_{\varepsilon, d})$ satisfies

$$N_d(k_{\varepsilon, d}) \leq 2 \exp \left\{ k_{\varepsilon, d} \left(2 + \ln \left(1 - d / \ln(\varepsilon) \right) \right) \right\}.$$

This shows, in particular, that the problem of integration for F_d is weakly tractable and that the CCS algorithm is weakly tractable for these classes.

One may argue that also the CCS algorithm is “mildly unstable” and one would prefer an algorithm with small operator norm, such as a cubature formula with positive weights that add up to 1. Indeed, we prove an analogue of Theorem 4 with a better dependence of the number of nodes.

Theorem 5. For each $d \in \mathbb{N}$ and $\varepsilon \in (0, 1]$ define

$$k_{\varepsilon, d}^* := \left\lceil \max \left\{ 4 d^{1/2}, \ln(1/\varepsilon) \right\} \right\rceil.$$

Then there exists a cubature rule $Q(k_{\varepsilon, d}^*, d)$ with positive weights that add up to 1 with error

$$e(k_{\varepsilon, d}^*, d) := \sup_{f \in F_d} |Q(k_{\varepsilon, d}^*, d)(f) - S_d(f)| \leq \varepsilon$$

and the number of function values $N_d^*(k_{\varepsilon,d}^*)$ used by $Q(k_{\varepsilon,d}^*, d)$ satisfies

$$N_d^*(k_{\varepsilon,d}^*) \leq \exp\left\{k_{\varepsilon,d}^* \left(1 + \ln\left(1 - d/\ln(\varepsilon)\right)\right)\right\}.$$

The proof is based on a constructive version of Tchakalov's Theorem due to Davis, see [6]. However, to construct these cubature formulas, one has to solve exponentially (in d) many linear systems of equations, each having exponentially many unknowns. So these methods can be applied only for small d . In contrast, the CCS Smolyak algorithm can be easily implemented.

1.5 Related results and open problems

- Considering the above remarks about the relation of Theorems 4 and 5, a natural question is whether the weak tractability of integration for F_d can be proved with a positive cubature formula which can be efficiently constructed. Additionally, we pose the same question for QMC algorithms, i.e. positive cubature formulas with equal weights. For recent surveys on QMC algorithms see [7, 8].

- The classes

$$F^d = \{f : [0, 1]^d \rightarrow \mathbb{R} \mid \|D^\alpha f\|_\infty \leq 1 \text{ for all } \alpha \in \mathbb{N}_0^d\}$$

were studied several times in the literature, also for the L_p approximation problem, see [11, 12, 13, 20, 21, 22, 33, 34]. Here we only mention that F_d from this paper is smaller than F^d and it is still *not* known whether integration is weakly tractable for the classes F^d .

- We do not know whether integration for the classes F_d from (14) is uniformly weakly tractable. See Siedlecki [24] for this stronger notion of tractability.
- There is an algorithm for the approximation problem that uses the same sparse grid $H(q, d)$ as well as interpolation by polynomials, see [3]. This algorithm is often applied, see, e.g., [1] and one may ask about tractability properties of this algorithm. We do not know whether the L_p approximation problem for the classes F_d from (14) is weakly tractable and, in particular, whether the weak tractability follows from properties of the Smolyak algorithm.
- The Smolyak algorithm was generalized to the weighted tensor product algorithm by Wasilkowski and Woźniakowski [31, 32] and these authors also proved tractability results for weighted tensor product problems; see also [22].

2 The proof

We start with computing the norms of Δ^ℓ and note that a similar (slightly weaker) result was already proved by Petras [23].

Lemma 6. For Δ^ℓ from (3) we have

$$\|\Delta^1\| = 1, \quad \|\Delta^2\| = \frac{2}{3} \quad \text{and} \quad \|\Delta^\ell\| = 1 + \frac{1}{4^{\ell-1} + 1}$$

for $\ell \geq 3$.

Proof. Recall that the norm of a quadrature rule is given by the sum of the absolute values of the used weights. Obviously, Δ^1 has only one weight equal to 1, so $\|\Delta^1\| = 1$. For Δ^2 it is an easy computation to check that there are three nodes with weights $b_1^2 = \frac{1}{6}$, $b_2^2 = -\frac{1}{3}$, $b_3^2 = \frac{1}{6}$, which gives

$$\|\Delta^2\| = \sum_{j=1}^3 |b_j^2| = \frac{2}{3}.$$

We now treat the case $\ell > 2$. Since we want to sum up the absolute values of the weights b_j^ℓ we first consider their signs. Clearly, $b_j^\ell = a_j^\ell > 0$ for even j .

For odd j we now show that $b_j^\ell < 0$ for all $\ell \geq 3$ and $j \leq m_\ell$. That is, we show that

$$a_{2j-1}^{\ell+1} < a_j^\ell$$

for $\ell \geq 2$ and (not necessarily odd) $j = 1, \dots, m_\ell$. For $j = 1, m_\ell$, noting that $m_{\ell+1} = 2m_\ell - 1$, this follows immediately from the formulas for the weights. So assume that $2 \leq j \leq m_\ell - 1$.

For $\ell = 2$, there is only the case $j = 2$ left. Direct computation shows

$$a_3^3 = \frac{2}{5} < \frac{2}{3} = a_2^2.$$

For $\ell \geq 3$, we use the absolutely convergent Fourier series

$$u(x) := \frac{\pi}{2} |\sin \pi x| = 1 - 2 \sum_{k=1}^{\infty} \frac{\cos 2kx\pi}{4k^2 - 1}.$$

Using this for $x = \frac{j-1}{m_\ell-1}$ and the weight formula (2) and abbreviating $u = u(x)$ we obtain

$$\begin{aligned} (m_\ell - 1)a_j^\ell - u &= -\frac{\cos(j-1)\pi}{(m_\ell - 1)^2 - 1} + 2 \sum_{k=\frac{m_\ell-1}{2}}^{\infty} \frac{\cos \frac{2k(j-1)\pi}{m_\ell-1}}{4k^2 - 1} \\ &= \frac{\cos(j-1)\pi}{(m_\ell - 1)^2 - 1} + 2 \sum_{k=\frac{m_\ell+1}{2}}^{\infty} \frac{\cos \frac{2k(j-1)\pi}{m_\ell-1}}{4k^2 - 1}. \end{aligned}$$

Note that

$$\left| 2 \sum_{k=\frac{m_\ell+1}{2}}^{\infty} \frac{\cos 2k\pi x}{4k^2-1} \right| \leq \sum_{k=\frac{m_\ell+1}{2}}^{\infty} \frac{2}{4k^2-1} = \sum_{k=\frac{m_\ell+1}{2}}^{\infty} \left(\frac{1}{2k-1} - \frac{1}{2k+1} \right) = \frac{1}{m_\ell}$$

for all $x \in \mathbb{R}$. This implies

$$|(m_\ell - 1)a_j^\ell - u| < \frac{1}{(m_\ell - 1)^2 - 1} + \frac{1}{m_\ell} = \frac{m_\ell - 1}{m_\ell(m_\ell - 2)} < \frac{1}{m_\ell - 2}$$

and thus

$$(m_\ell - 1)a_j^\ell > u - \frac{1}{m_\ell - 2}. \quad (15)$$

Similarly, noting that $x = \frac{j-1}{m_\ell-1} = \frac{2j-2}{m_{\ell+1}-1}$, we obtain that

$$2(m_\ell - 1)a_{2j-1}^{\ell+1} = (m_{\ell+1} - 1)a_{2j-1}^{\ell+1} < u + \frac{1}{m_{\ell+1} - 2} = u + \frac{1}{2m_\ell - 3} < u + \frac{1}{2(m_\ell - 2)}. \quad (16)$$

Recall that our aim is to show that $a_{2j-1}^{\ell+1} < a_j^\ell$ which, thanks to (15) and (16), is certainly satisfied if

$$u > \frac{5}{2(m_\ell - 2)}.$$

Using $m_\ell \geq 5$ and $\sin x \geq \frac{2\sqrt{2}x}{\pi}$ for $x \in [0, \pi/4]$, we can conclude this from

$$u = \frac{\pi}{2} \left| \sin \frac{(j-1)\pi}{m_\ell-1} \right| \geq \frac{\pi}{2} \sin \frac{\pi}{m_\ell-1} \geq \frac{\pi\sqrt{2}}{m_\ell-1} > \frac{5}{m_\ell-1} > \frac{5}{2(m_\ell-2)}.$$

This finally shows $a_{2j-1}^{\ell+1} < a_j^\ell$ for all $\ell \geq 2$ and $j = 1, \dots, m_\ell$ and, consequently, that $b_j^\ell < 0$ for all $\ell \geq 3$ and all odd j .

Now we can compute the norm

$$\|\Delta^\ell\| = \sum_{j=1}^{m_\ell} |b_j^\ell| = \sum_{j=1}^{\frac{m_\ell-1}{2}} a_{2j}^\ell - \sum_{j=1}^{\frac{m_\ell+1}{2}} a_{2j-1}^\ell + \sum_{j=1}^{m_{\ell-1}} a_j^{\ell-1}.$$

Using twice that the weights of one CC-rule add up to 1 we obtain

$$\|\Delta^\ell\| = 2 \sum_{j=1}^{\frac{m_\ell-1}{2}} a_{2j}^\ell = 2 \sum_{j=1}^{2^{\ell-2}} \frac{1}{2^{\ell-1}} \left(1 + \frac{1}{4^{\ell-1} - 1} - 2 \sum_{k=1}^{2^{\ell-2}-1} \frac{\cos \frac{2k(2j-1)\pi}{2^{\ell-1}}}{4k^2 - 1} \right).$$

Simplifying and changing the order of summation yields

$$\|\Delta^\ell\| = 1 + \frac{1}{4^{\ell-1} - 1} + \frac{1}{2^{\ell-3}} \sum_{k=1}^{2^{\ell-2}-1} \frac{1}{4k^2 - 1} \sum_{j=1}^{2^{\ell-2}} \cos \frac{k(2j-1)\pi}{2^{\ell-2}}.$$

Since the inner sum is always zero, we finally arrive at

$$\|\Delta^\ell\| = 1 + \frac{1}{4^{\ell-1} - 1}.$$

□

Now we are able to prove our explicit bound on the norm of the Smolyak algorithm.

Proposition 7. For every $k \in \mathbb{N}_0$ and $d \in \mathbb{N}$ we have

$$\|A(d+k, d)\| \leq \binom{d+k}{d} \leq e^k \left(1 + \frac{d}{k}\right)^k.$$

Proof. The second inequality is proven by

$$\binom{d+k}{d} \leq \frac{(d+k)^k}{k!} \leq \left(\frac{e(d+k)}{k}\right)^k,$$

where we used Stirling's approximation of the factorial.

To prove the first inequality, we show that

$$M(k, d) := \max_{0 \leq \ell \leq k} \|A(d+\ell, d)\| \leq \binom{d+k}{d}$$

by induction on d . For $d = 1$ we obviously have

$$M(k, 1) := \|A(1+k, 1)\| = \|U^{k+1}\| = 1 \leq \binom{1+k}{1}$$

for every $k \in \mathbb{N}_0$. For $d \geq 1$ let us now assume $M(k, d) \leq \binom{d+k}{d}$ for all $k \in \mathbb{N}_0$ and recall that, for $d, k \in \mathbb{N}_0$, we have

$$\sum_{\ell=0}^k \binom{d+\ell}{d} = \binom{d+k+1}{d+1}.$$

Then we obtain by Lemma 6 that

$$\begin{aligned}
\|A(d+1+k, d+1)\| &\leq \sum_{\ell=1}^{k+1} \|A(d+1+k-\ell, d)\| \cdot \|\Delta^\ell\| \\
&\leq \sum_{\ell=1}^{k+1} M(k+1-\ell, d) \|\Delta^\ell\| \\
&= M(k, d) + \frac{2}{3} M(k-1, d) + \sum_{\ell=3}^{k+1} \frac{4^{\ell-1}}{4^{\ell-1}-1} M(k+1-\ell, d) \\
&= \sum_{\ell=1}^{k+1} M(k+1-\ell, d) - \frac{1}{3} M(k-1, d) \\
&\quad + \sum_{\ell=3}^{k+1} \frac{1}{4^{\ell-1}-1} M(k+1-\ell, d) \\
&\leq \sum_{\ell=0}^k M(\ell, d) - M(k-1, d) \left(\frac{1}{3} - \sum_{\ell=3}^{k+1} \frac{1}{4^{\ell-1}-1} \right),
\end{aligned}$$

where we have used that $M(k+1-\ell, d) \leq M(k-1, d)$ for $k = 3, \dots, k+1$. Noting that

$$\sum_{\ell=3}^{k+1} \frac{1}{4^{\ell-1}-1} = \sum_{\ell=0}^{k-2} \frac{1}{4^{\ell+2}-1} \leq \sum_{\ell=0}^{k-2} \frac{1}{4^{\ell+1}} \leq \frac{1}{3},$$

we finally obtain

$$\|A(d+1+k, d+1)\| \leq \sum_{\ell=0}^k M(\ell, d) \leq \sum_{\ell=0}^k \binom{d+\ell}{d} = \binom{d+1+k}{d+1}.$$

Writing this inequality down with k replaced by ℓ and taking the maximum over $\ell = 0, 1, \dots, k$ on both sides leads to

$$M(k, d+1) \leq \max_{0 \leq \ell \leq k} \binom{d+1+\ell}{d+1} = \binom{d+1+k}{d+1}$$

and concludes the induction step and the proof. □

Note that Proposition 1 holds also for the Smolyak algorithm that is based on other one-dimensional quadrature rules as long as

$$\|\Delta^1\| \leq 1 \quad \text{and} \quad \sum_{\ell=2}^{\infty} (\|\Delta^\ell\| - 1) \leq 0.$$

To conclude our main result, Theorem 4, we additionally need a bound on the error of approximation by polynomials. We prove that d -dimensional C^∞ functions with directional derivatives of all orders bounded by one can be arbitrarily well approximated by polynomials of total degree of order \sqrt{d} . This result was already proven by the authors and H. Woźniakowski in [12], but we state the proof here again for completeness. Let \mathcal{P}_k be the space of polynomials of degree k .

Proposition 8. Let $f \in F_d$ and $k \in \mathbb{N}$. Then

$$\inf_{p \in \mathcal{P}_{k-1}} \|f - p\|_\infty \leq \sqrt{\frac{1}{2\pi k}} \left(\frac{e\sqrt{d}}{2k} \right)^k.$$

Proof. Consider the Taylor polynomial for $f \in F_d$ of order $k - 1$ about the point $x^* = (1/2, \dots, 1/2)$ which can be written as

$$T_{k-1}(x) = \sum_{\ell=0}^{k-1} \frac{f^{(\ell)}(x^*)(x - x^*)^\ell}{\ell!} \quad \text{for all } x \in [0, 1]^d.$$

Here we use the standard notation $A(x^\ell) = A(x, \dots, x)$ for the evaluation of an ℓ -linear map on the diagonal. Note that we consider here $f^{(\ell)}(x^*)$ as an ℓ -linear map. It is well-known that the error of the approximation of f by T_{k-1} can be written as

$$f(x) - T_{k-1}(x) = k \int_0^1 (1-t)^{k-1} \frac{f^{(k)}(x^* + t(x - x^*))(x - x^*)^k}{k!} dt,$$

which implies

$$\begin{aligned} |f(x) - T_{k-1}(x)| &\leq \frac{1}{(k-1)!} \int_0^1 (1-t)^{k-1} dt \left(\max_{\theta \in S^{d-1}} \|D_\theta^k f\|_\infty \right) \|x - x^*\|_2^k \\ &\leq \frac{1}{2^k k!} d^{k/2}. \end{aligned}$$

An application of Stirling's formula proves the result since $T_{k-1} \in \mathcal{P}_{k-1}$. □

We combine Propositions 7 and 8 to obtain the first part of our main result. To ease the calculations we use the trivial bound $\inf_{p \in \mathcal{P}_{2k+1}} \|f - p\|_\infty \leq \inf_{p \in \mathcal{P}_{2k-1}} \|f - p\|_\infty$. Recall that

$$e(k, d) := \sup_{f \in F_d} |A(d+k, d)(f) - S_d(f)|.$$

Using that $A(d+k, d)$ is exact for all polynomials of total degree at most $2k+1$, see [16, 18], we have

$$\begin{aligned} e(k, d) &\leq \sup_{f \in F_d} \inf_{p \in \mathcal{P}_{2k+1}} \|f - p\|_\infty \left(1 + \|A(d+k, d)\|\right) \\ &\leq \sqrt{\frac{1}{4\pi k}} \left(\frac{e\sqrt{d}}{4k}\right)^{2k} \left(1 + e^k \left(1 + \frac{d}{k}\right)^k\right) \leq \sqrt{\frac{1}{\pi k}} \left(\frac{e\sqrt{d}}{4k}\right)^{2k} e^k \left(1 + \frac{d}{k}\right)^k \\ &\leq \frac{1}{\sqrt{\pi k}} \left(\frac{e^3}{16}\right)^k \left(\frac{d}{k^2} + \frac{d^2}{k^3}\right)^k \leq \frac{1}{\sqrt{\pi k}} \left(\frac{e^3 d}{8k^2} \max\left\{1, \frac{d}{k}\right\}\right)^k. \end{aligned}$$

This shows that with

$$k_{\varepsilon, d} := \left\lceil \max\left\{3d^{2/3}, \ln(1/\varepsilon)\right\} \right\rceil$$

we have $e(k_{\varepsilon, d}, d) \leq \varepsilon$, which is the first part of Theorem 4.

It remains to prove the bound on the number of function values $N_d(k_{\varepsilon, d})$ that are used by the Smolyak algorithm $A(d+k_{\varepsilon, d}, d)$. For this we use the following bound of Wasilkowski and Woźniakowski.

Lemma 9 ([30], Lemma 7). The number of function values used by the Smolyak algorithm $A(d+k, d)$ that is based on the one-dimensional quadrature rules from (1) satisfies

$$N_d(k) \leq 2(2e)^k \left(1 + \frac{d}{k}\right)^k$$

for all $k, d \in \mathbb{N}$, and thus

$$\ln(N_d(k)) \leq \ln 2 + k \left(\ln(2e) + \ln\left(1 + \frac{d}{k}\right)\right).$$

Proof. Since our m_ℓ 's satisfy $m_\ell \leq 2^\ell - 1$ and the used nodes are nested, we use equation (43) of [30] with $F_0 = 1$, $F = 2$ and $q = d+k$. This gives

$$N_d(k) \leq 2^{k+1} \binom{d+k-1}{d-1} \leq 2(2e)^k \left(1 + \frac{d}{k}\right)^k$$

by Stirling's formula. □

From this we obtain

$$\begin{aligned} \ln(N_d(k_{\varepsilon,d})) &\leq \ln 2 + k_{\varepsilon,d} \left(\ln(2e) \right. \\ &\quad \left. + \min\left\{ \ln(1 + (1/3) d^{1/3}), \ln(1 + d \ln(1/\varepsilon)^{-1}) \right\} \right) \\ &\leq \ln 2 + k_{\varepsilon,d} \left(2 + \ln\left(1 - \frac{d}{\ln(\varepsilon)}\right) \right), \end{aligned}$$

which is the second part of Theorem 4.

The proof of Theorem 5 proceeds similarly, so we only sketch the necessary modifications. It follows from [6] that for all $k, d \in \mathbb{N}$ there exists a cubature formula $Q(k, d)$ with positive weights, exactness k and such that the number of function values $N_d^*(k)$ satisfies the Tschakalov bound

$$N_d^*(k) \leq \binom{d+k}{d} \leq e^k \left(1 + \frac{d}{k}\right)^k. \quad (17)$$

This implies that $\|Q(k, d)\| = 1$ which can now be used instead of Proposition 7. So, we obtain for the error

$$e(k, d) \leq \sup_{f \in F_d} \inf_{p \in \mathcal{P}_k} \|f - p\|_{\infty} \left(1 + \|Q(k, d)\|\right) \leq \sqrt{\frac{2}{\pi k}} \left(\frac{e\sqrt{d}}{2k}\right)^k,$$

which is smaller than ε for $k = k_{\varepsilon,d}^*$ as in Theorem 5. Finally, the bound on $N_d^*(k_{\varepsilon,d}^*)$ in Theorem 5 now follows from (17).

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