SIMPLE CUBATURE FORMULAS WITH HIGH POLYNOMIAL EXACTNESS

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ABSTRACT. We study cubature formulas for d-dimensional integrals with arbitrary weight function of tensor product form. We present a construction that yields a high polynomial exactness: for fixed degree the number of knots depends on the dimension in an order-optimal way. The cubature formulas are universal: the order of convergence is almost optimal for two different scales of function spaces. The construction is simple: a small number of arithmetical operations is sufficient to compute the knots and the weights of the formulas.

1. Introduction

We study (sequences of) cubature formulas

$$Q_n(f) = \sum_{i=1}^{n} a_i \, f(\mathbf{x}_i), \qquad a_i \in \mathbb{R},\ \ \mathbf{x}_i \in \Omega, \tag{1}$$

for d-dimensional integrals

$$I_d(f) = \int_\Omega f(\mathbf{x}) \, \varrho(\mathbf{x}) \, d\mathbf{x}. \tag{2}$$

Concerning the integral we always assume

$$\Omega = \Omega_1 \times \cdots \times \Omega_d \tag{3}$$

with possibly unbounded intervals $\Omega_j \subset \mathbb{R}$ and the tensor product form

$$\varrho(\mathbf{x}) = \varrho_1(x_1) \dots \varrho_d(x_d) \tag{4}$$

of the weight function ϱ.

We present a construction with the following properties:

Simplicity. The formulas Q_n can be easily computed for arbitrary dimensions d and weight functions ϱ of the form (4). We need $\mathcal{O}(n)$ arithmetic operations to compute the knots and weights of Q_n from suitable univariate quadrature formulas.

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High Polynomial Exactness. A small number of knots is sufficient to integrate all d-variate polynomials of a given degree exactly. We need

$$n \approx 2^k/k! \cdot d^k \tag{5}$$

knots for degree $2k+1$ of exactness 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. For fixed d and large k the number of knots is of the order $k^d \cdot (\log k)^{d-1}$. The well known lower bound is of the order k^d.

Universality. The order of convergence is almost optimal for many different smoothness classes. Assume that Ω is bounded. If f has bounded derivatives up to order r then

$$|I_d(f) - Q_n(f)| = \mathcal{O}\Big(n^{-r/d} \cdot (\log n)^{(d-1)(r/d+1)}\Big). \tag{6}$$

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

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

These two estimates are optimal – up to logarithmic factors – in both smoothness scales. The bounds (6) and (7) hold for all $r \in \mathbb{N}$, 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.[1]

We assume $\varrho_j \geq 0$ and integrability of all polynomials, although these assumptions can be relaxed. These conditions, together with (3) and (4), form what we call the general case in the following, see Sections 3 and 5. In this case the construction is based on Gaussian quadrature formulas for every ϱ_j.

We also consider the particular case of symmetric weight functions ϱ_j and bounded domains Ω, see Section 4. In this case the construction is based on Chebyshev knots of the second kind together with the endpoints. Here only the weights of the cubature formulas (1) depend on ϱ.

In this paper the focus is on polynomial exactness. Error bounds and numerical experiments were already presented in Novak and Ritter (1996, 1997) and Novak, Ritter, Schmitt, and Steinbauer (1997).

Let $\mathbb{P}(\ell, d)$ be the space of all polynomials in d variables of (total) degree at most ℓ. A cubature formula Q_n has a degree ℓ of exactness if

$$Q_n(f) = I_d(f), \qquad \forall\, f \in \mathbb{P}(\ell, d).$$

We define

$$N_{\min}(\ell, d)$$

[1] There exist several definitions of universality. Generally spoken, universality means that a quadrature formula, or a sequence of quadrature formulas, is good for many different classes of functions. See, in particular, Brass (1988), Petras (1996), and Temlyakov (1991).

to be the minimal number n of knots needed by any cubature formula Q_n of degree ℓ of exactness. Here we assume that the region Ω and the weight function ϱ are given and fixed.

The numbers $N_{\min}(\ell, d)$ and corresponding cubature formulas are only known in exceptional cases, see, e.g., Schmid (1983) and Cools (1997). Thus one is interested in upper and lower bounds for this quantity. It is well known that

$$N_{\min}(\ell, d) \leq \dim \mathbb{P}(\ell, d), \tag{8}$$

where

$$\dim \mathbb{P}(\ell, d) = \binom{\ell + d}{d}.$$

This upper bound can be achieved by cubature formulas with positive weights a_i. Moreover,

$$\dim \mathbb{P}(\lfloor \ell/2 \rfloor, d) \leq N_{\min}(\ell, d). \tag{9}$$

In many special cases improvements of these bounds are known. The results of this paper imply new upper bounds. We construct, in a simple and explicit way, cubature formulas Q_n with degree ℓ of exactness such that n is not "much" larger than $N_{\min}(\ell, d)$.

One is often interested in cubature formulas with knots inside the domain and positive weights. While $\mathbf{x}_i \in \Omega$ is always satisfied by our method, we usually have positive and negative weights. However, we have

$$\|Q_n\| = \sum_{i=1}^{n} |a_i| = \mathcal{O}((\log n)^{d-1})$$

which is important to prove error bounds and for the stability. The norms $\|Q_n\|$ are much smaller in the Chebyshev case, compared to the Gaussian case.

Suppose that all weight functions ϱ_j are symmetric. If one is only interested in polynomial exactness and simplicity, then the above constructions, based either on Chebyshev or Gaussian knots, can be improved, see Section 6. The number of knots achieves the optimal order in both directions. More precisely, we need $n \approx 2^d/d! \cdot k^d$ knots for degree $2k+1$ of exactness if d is fixed and k is large; in the dual situation we obtain (5), as previously. However, we do not have error bounds, since $\|Q_n\|$ might be too large.

In the remaining part of the introduction we discuss several other constructions of cubature formulas with high polynomial exactness. We consider the case of odd degree $2k+1$ of exactness.

Product Gaussian formulas. Product Gaussian rules are easy to construct. However, the number of knots is m^d with $m \in \mathbb{N}$. Therefore such an "exponential" method cannot really be applied if d is large, say $d = 25$.

One needs $(k+1)^d$ knots for degree $2k+1$ of exactness. For fixed k and large d this exponential growth is very bad. If d is fixed, however, the number of the knots is about k^d, compared to the lower bound $1/d! \cdot k^d$, i.e., one gets the optimal order.

Instead of (6) the optimal order $n^{-r/d}$ of the error is achieved by Gaussian product rules. However, instead of (7) one also has errors of order $n^{-r/d}$, which is rather poor.

Constructive versions of Tchakalov's Theorem. The Tchakalov bound (8) can be achieved by a constructive method, see Davis (1967). Cools (1992) uses ideal theory to obtain the improved bound

$$N_{\min}(2k+1,d) \le \binom{2k+1+d}{d} - d\binom{k+d}{d} \tag{10}$$

for the number of knots. Both approaches yield formulas with positive weights. However, one has to solve about k^d linear systems of equations, each having about k^d unknowns. So these methods can be applied only for small d.

For fixed k the number of knots increases like d^{2k+1} which is not optimal, while for fixed d one achieves the optimal order k^d.

The error bounds coincide with the ones for product Gaussian formulas, i.e., one gets $n^{-r/d}$ in both smoothness scales.

Fully symmetric formulas. Cubature formulas with high polynomial exactness are not often used if d is large, say $d > 5$. One major exception is the class of fully symmetric rules for the fully symmetric case, where

$$\varrho_1 = \cdots = \varrho_d$$

and

$$\varrho_j(x) = \varrho_j(-x).$$

Fully symmetric cubature formulas were developed by Lyness (1965a, 1965b), McNamee and Stenger (1967), Genz (1986), Cools and Haegemans (1994), Capstick and Keister (1996), Genz and Keister (1996) and other authors. The best results with respect to polynomial exactness are obtained by Genz (1986) and Genz and Keister (1996). The methods, at least some of them, are simple in the sense that the knots and weights can be computed easily.

We show that the fully symmetric formulas from Genz (1986) and Genz and Keister (1996) are of the Smolyak form (13). In fact, our construction in Section 6 is a generalization of the approach from the latter two papers to the symmetric case.

Unfortunately, error bounds are not known for these methods. The problem is that there are no general bounds for the norms $\|Q_n\|$. These numbers can of course be computed in each special case. The numerical values are rather promising, at least in some cases, and it would be very interesting to have general upper bounds.

Example. Let us compare several approaches discussed above. We consider dimension $d = 25$ and degree $\ell = 7$ of exactness. Due to the lower bound (9),

$$n \geq 3276$$

knots are needed by every cubature formula that is exact on $\mathbb{P}(7, 25)$. Our constructions in Sections 4–6 need

$$n = 22\,201, \quad 24\,751, \quad 22\,151$$

knots, respectively. In the fully symmetric case, the number 22 151 is also achieved by Genz (1986), see Remark 10 for further discussion and improvements. A product Gaussian formula requires

$$n = 4^{25} \geq 10^{16}$$

knots. The Tchakolov bound (8) yields

$$n = 3\,365\,856,$$

and by (10) this number is reduced to

$$n = 3\,283\,956.$$

Hence these upper bounds are much too large. The same comparison leads to different results if d is small and ℓ is large. We consider dimension $d = 5$ and degree $\ell = 17$ of exactness. Due to the lower bound (9),

$$n \geq 1\,287$$

knots are needed by every cubature formula that is exact on $\mathbb{P}(17, 5)$. Our constructions in Sections 4–6 need

$$n = 51\,713, \quad 187\,552, \quad 13\,073$$

knots, respectively. A product Gaussian formula requires

$$n = 9^5 = 59\,049$$

knots. The Tchakolov bound yields

$$n = 26\,334$$

and by (10) this number is reduced to

$$n = 19\,899.$$

Many more numbers can be found in our Tables 1–3. These tables also show that we only obtain a reasonably small n if the dimension and the degree are not too large. If, for example, the dimension is 25 and the degree is 17 then all our methods use $n > 10^{10}$ function values. In this case the dimension of the space of exactness is about $2.5 \cdot 10^{11}$ and the lower bound is about $1.4 \cdot 10^7$.

Based on results from Section 3 the periodic case (with trigonometric polynomials instead of algebraic polynomials) is studied in Cools, Novak, and Ritter (1997), with surprisingly different results.

2. The Method

We construct interpolatory cubature formulas to compute the integral (2) as follows. First we select interpolatory quadrature formulas $U_j^1, U_j^2, \ldots$ to compute the one-dimensional integrals

$$\int_{\Omega_j} f(x)\, \varrho_j(x)\, dx.$$

These formulas should have the following two properties: The formula U_j^i is exact for all univariate polynomials of degree m_i, where

$$m_1 = 1, \qquad m_2 \geq 3, \qquad \text{and} \qquad m_{i+1} - m_i \geq m_i - m_{i-1}. \tag{11}$$

The number n_i of knots that are used by U_j^i satisfies

$$n_i \leq m_i + 1. \tag{12}$$

By (12) the weights of U_j^i are uniquely determined by its knots. Formulas with this property often are called interpolatory quadrature formulas.

For simplicity we assume in this paper that the numbers m_i and n_i do not depend on the coordinate j. The formula U_j^i, however, may depend on j.

A product formula $U_1^{i_1} \otimes \cdots \otimes U_d^{i_d}$ needs $n_{i_1} \ldots n_{i_d}$ function values, sampled on a grid. The Smolyak formulas $A(q,d)$ are linear combinations of product formulas with the following key properties. Only products with a relatively small number of knots are used and the linear combination is chosen in such a way that the interpolation property for $d = 1$ is preserved for $d > 1$. The formula $A(q,d)$ is defined by

$$A(q,d) = \sum_{q-d+1 \leq |\mathbf{i}| \leq q} (-1)^{q-|\mathbf{i}|} \cdot \binom{d-1}{q-|\mathbf{i}|} \cdot (U_1^{i_1} \otimes \cdots \otimes U_d^{i_d}), \tag{13}$$

where $q \geq d$, $\mathbf{i} \in \mathbb{N}^d$, and $|\mathbf{i}| = i_1 + \cdots + i_d$. Henceforth we use

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

to denote the total number of knots that are used by $A(q,d)$. Obviously

$$n(q,d) \leq \tilde{n}(q,d)$$

where

$$\tilde{n}(q,d) = \sum_{q-d+1 \leq |\mathbf{i}| \leq q} n_{i_1} \ldots n_{i_d}.$$

Note that $n(q,d)$ may be much smaller than $\tilde{n}(q,d)$ if different grids contain common points.

Numerical integration with the Smolyak construction was already studied in Smolyak (1963). Other papers include Genz (1974), Temlyakov (1987), Delvos (1990), Paskov (1993), Ritter, Wasilkowski, and Woźniakowski (1993), Bonk (1994), Lyness and Sloan (1995), Wasilkowski and Woźniakowski (1995), Frank and Heinrich (1996), and Gerstner, Griebel (1998). In some of these papers the stress is on the numerical integration of periodic functions. We also mention Novak and Ritter (1996, 1997) where the stress is on error bounds and numerical results. For further numerical results and applications see also Novak, Ritter, Schmitt and Steinbauer (1997). Modifications of the Smolyak construction even work for infinite dimensional Wiener integrals, see Novak, Ritter, and Steinbauer (1998).

3. General Estimates

Let $A(q,d)$ denote the cubature formula (13) with univariate formulas U_j^i. The following analysis is only based on the sequences $(n_i)_i$ and $(m_i)_i$. The latter sequence is chosen such that U_j^i has a degree m_i of exactness and (11) holds. We stress that m_i need not be the maximal degree of exactness, i.e., we do not require

$$U_j^i(f) \neq \int_{\Omega_j} f(x)\, \varrho_j(x)\, dx$$

for some $f \in \mathbb{P}(m_i+1,1)$.

Lemma 1. *Assume $m_i \leq m_{i+1}$. Then*

$$A(q,d)(f) = I_d(f)$$

for all polynomials

$$f \in \sum_{|\mathbf{i}|=q} (\mathbb{P}(m_{i_1},1) \otimes \cdots \otimes \mathbb{P}(m_{i_d},1)) =: E(q,d).$$

Proof. For specific formulas $A(q,d)$ the proof is given in Novak and Ritter (1996). The same proof applies here, since the spaces $\mathbb{P}(m_i,1)$ of exactness of U_j^i are nested. For convenience of the reader we include the argument which is via induction over d. For $d=1$ we have $A(q,1)=U_1^q$ and the statement follows. For the multivariate case we use the fact that $A(q,d+1)$ can be written in terms of the $A(\ell,d)$, we have

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

Here we put $U_j^0 = 0$.

The induction step is as follows. Assume that

$$f = f_{i_1} \otimes \cdots \otimes f_{i_{d+1}}, \qquad f_{i_k} \in \mathbb{P}(m_{i_k},1),$$

with $|\mathbf{i}|=q$ and $i_1+\cdots+i_d=m$ whence $m+i_{d+1}=q$. Then

$$A(q,d+1)(f) = \sum_{\ell=d}^{q-1} A(\ell,d)(f_{i_1} \otimes \cdots \otimes f_{i_d}) \cdot (U_{d+1}^{q-\ell} - U_{d+1}^{q-\ell-1})(f_{i_{d+1}}).$$

Since

$$U_{d+1}^{q-\ell}(f_{i_{d+1}}) = U_{d+1}^{q-\ell-1}(f_{i_{d+1}}) = \int_{\Omega_{d+1}} f_{i_{d+1}}(x) \varrho_{d+1}(x)\, dx, \qquad d \leq \ell \leq m-1,$$

and

$$A(\ell,d)(f_{i_1}\otimes\cdots\otimes f_{i_d}) = I_d(f_{i_1}\otimes\cdots\otimes f_{i_d}), \qquad m\le \ell\le q-1,$$

we obtain

$$\begin{aligned} A(q,d+1)(f) &= \sum_{\ell=m}^{q-1} I_d(f_{i_1}\otimes\cdots\otimes f_{i_d})\cdot (U_{d+1}^{q-\ell}-U_{d+1}^{q-\ell-1})(f_{i_{d+1}}) \\ &= I_d(f_{i_1}\otimes\cdots\otimes f_{i_d})\cdot U_{d+1}^{q-m}(f_{i_{d+1}}) = I_{d+1}(f) \end{aligned}$$

as claimed. □

For the classical spaces $\mathbb{P}(\ell,d)$ we obtain the following result.

Theorem 1. *Assume* (11) *and let* $m_0=-1$. *Define* $\ell(q,d)$ *by*

$$\ell(q,d) = (m_{\sigma-1}+1)\cdot(d-(\tau+1)) + (m_\sigma+1)\cdot(\tau+1) - 1$$

where

$$q = \sigma d + \tau$$

for some $\sigma\in\mathbb{N}$ *and* $\tau\in\{0,\dots,d-1\}$. *Then* $A(q,d)$ *has degree* $\ell(q,d)$ *of exactness.*

Proof. Due to Lemma 1 it is sufficient to verify that

$$\mathbb{P}(\ell(q,d),d)\subset E(q,d) \tag{14}$$

for every $q\ge d$ and $d\in\mathbb{N}$. If $d=1$ then $\ell(q,1)=m_q$ which yields (14). Inductively we proceed as follows.

Since $\ell(d+1,d+1)=1$ and $\mathbb{P}(1,d+1)\subset E(d+1,d+1)$, we assume $q>d+1$. Consider a monomial from $\mathbb{P}(\ell(q,d+1),d+1)$,

$$(x_1,\dots,x_d)^{\boldsymbol{\alpha}}\cdot x_{d+1}^{\beta} = \prod_{i=1}^{d} x_i^{\alpha_i}\cdot x_{d+1}^{\beta},$$

and assume

$$|\boldsymbol{\alpha}|+\beta\le \ell(q,d+1).$$

Define $j\in\mathbb{N}$ by

$$\beta\in[m_{j-1}+1,m_j].$$

Clearly

$$|\boldsymbol{\alpha}|\le \ell(q,d+1)-m_{j-1}-1.$$

It remains to show that

$$\ell(q,d+1)-m_{j-1}-1\le \ell(q-j,d), \tag{15}$$

since then, by hypothesis,

$$(x_1,\dots,x_d)^{\boldsymbol{\alpha}}\in \mathbb{P}(m_{i_1},1)\otimes\cdots\otimes\mathbb{P}(m_{i_d},1)$$

for some $\mathbf{i}\in\mathbb{N}^d$ with $|\mathbf{i}|\le q-j$ and finally

$$(x_1,\dots,x_d)^{\boldsymbol{\alpha}}\cdot x_{d+1}^{\beta}\in \mathbb{P}(m_{i_1},1)\otimes\cdots\otimes\mathbb{P}(m_{i_d},1)\otimes\mathbb{P}(m_j,1)\subset E(q,d+1).$$

Assume that

$$q = \sigma(d+1) + \tau$$

with $\sigma \in \mathbb{N}$ and $\tau \in \{0, \dots, d\}$ as well as

$$q - j = \widetilde{\sigma} d + \widetilde{\tau}$$

with $\widetilde{\sigma} \in \mathbb{N}$ and $\widetilde{\tau} \in \{0, \dots, d-1\}$. If we plug in the definition, then (15) has the form

$$m_{\sigma-1}(d-\tau) + m_{\sigma}(\tau+1) \leq m_{j-1} + m_{\widetilde{\sigma}-1}(d-\widetilde{\tau}-1) + m_{\widetilde{\sigma}}(\widetilde{\tau}+1).$$

This inequality, which we now have to prove, has the form

$$\sum_{i=1}^{N} m_{j_i} \leq \sum_{i=1}^{N} m_{k_i}, \tag{16}$$

where

$$N = d + 1$$

as well as

$$\sum_{i=1}^{N} j_i = (d-\tau)\cdot(\sigma-1) + (\tau+1)\cdot\sigma = q - d$$

and

$$\sum_{i=1}^{N} k_i = (j-1) + (d-\widetilde{\tau}-1)\cdot(\widetilde{\sigma}-1) + (\widetilde{\tau}+1)\cdot\widetilde{\sigma} = q - d.$$

Thus the number of terms and also the sum of the indices coincide on both sides of the inequality (16). The inequality follows by our convexity assumption (11) and the fact that on the left side of (16) only two consecutive indices, $\sigma - 1$ and σ, appear. □

Note that (11) implies $m_i \geq 2i - 1$ for every $i \in \mathbb{N}$. The sequence $m_i = 2i - 1$ will play a special role, see Section 6.

Corollary 1. *Assume* (11)*. Then $A(q,d)$ has (at least) a degree $2\,(q-d)+1$ of exactness.*

Now we derive 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.,

$$v_n \approx w_n \qquad \text{iff} \qquad \lim_{n\to\infty} v_n/w_n = 1.$$

Furthermore, we write

$$v_n \preceq w_n \qquad \text{iff} \qquad \limsup_{n\to\infty} v_n/w_n \leq 1.$$

We study the growth of $n(k+d,d)$ for fixed k as d tends to infinity. We use X_j^i to denote the set of knots that are used by U_j^i. Recall that $n_i = \#X_j^i$. Since $n(d,d) = n_1^d$ we require

$$n_1 = 1. \tag{17}$$

Since $m_1 = 1$ this implies that every U_j^1 is a one-point Gaussian formula. It turns out that $X_j^2 \setminus X_j^1$ should be small in order to obtain a slowly growing sequence $n(k+d,d)$ in d. Hence we require

$$\#(X_j^2 \setminus X_j^1) = 2 \tag{18}$$

for $j = 1, \dots, d$. We observe that U_j^2 is a two-point Gaussian formula if $X_j^1 \not\subset X_j^2$, since $m_2 \geq 3$. For symmetric weight functions ϱ_j one may take $n_2 = 3$ and an arbitrary symmetric set $X_j^2 \supset X_j^1$ to obtain $m_2 = 3$.

Lemma 2. *Assume* (17) *and* (18). *For $d \to \infty$ and fixed k*

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

and

$$\tilde{n}(k+d,d) \preceq \frac{3^k}{k!} \cdot d^k.$$

If $X_j^1 \not\subset X_j^2$ for every j, then $\tilde{n}(k+d,d) \approx n(k+d,d)$.

Proof. The cubature formula $A(q,d)$ is based on the sparse grid

$$H(q,d) = \bigcup_{q-d+1 \leq |\mathbf{i}| \leq q} X_1^{i_1} \times \cdots \times X_d^{i_d}. \tag{19}$$

Put $X_0 = \emptyset$ to obtain

$$H(k+d,d) \supset \bigcup_{|\mathbf{i}|=k+d,\ \mathbf{i} \leq 2} \left(X_1^{i_1} \setminus X_1^{i_1-1}\right) \times \cdots \times \left(X_d^{i_d} \setminus X_d^{i_d-1}\right).$$

Inequalities like $\mathbf{i} \leq 2$ with $\mathbf{i} \in \mathbb{N}^d$ are understood to hold in each coordinate. Hence

$$n(k+d,d) \geq \binom{d}{k} \cdot 2^k$$

by (17) and (18), and the lower bounds for $n(q,d) \leq \tilde{n}(q,d)$ follow.

If $\mathbf{x} = (x_1, \dots, x_d) \in H(k+d,d)$ then at most k coordinates of $\mathbf{x}$ do not belong to the respective set X_j^1. Fix $J \subset \{1, \dots, d\}$ with cardinality $\#J = \nu \leq k$. Assume that $\mathbf{x} \in H(k+d,d)$ with $x_j \notin X_j^1$ iff $j \in J$. If $\nu = k$ then

$$x_j \in X_j^2 \setminus X_j^1$$

for every $j \in J$, and therefore (17) and (18) yield

$$\#\{\mathbf{x} \in H(k+d,d) \mid x_j \notin X_j^1 \text{ iff } j \in J\} \leq 2^k.$$

If $\nu < k$ then

$$x_j \in \bigcup_{i=1}^{k} X_j^i$$

for every $j \in J$, and therefore

$$\#\{\mathbf{x} \in H(k+d,d) \mid x_j \notin X_j^1 \text{ iff } j \in J\} \leq \Big(\sum_{i=1}^{k} n_i\Big)^k =: c_k.$$

We obtain

$$n(k+d,d) \leq \sum_{\nu=0}^{k-1} \binom{d}{\nu} \cdot c_k + \binom{d}{k} \cdot 2^k \leq k \cdot d^{k-1} \cdot c_k + \binom{d}{k} \cdot 2^k.$$

Hereby the upper bound for $n(q,d)$ follows. A straigtforward modification yields the upper bounds for $\tilde{n}(q,d)$. □

Remark 1. The knots and weights of the formulas $A(q,d)$ can be computed by a single algorithm with inputs q and d with a small number of arithmetic operations. Let $\operatorname{cost}(q,d)$ denote the respective computational cost. Of course, one has to specify the numbers n_i and quadrature formulas U_j^i. We assume that all knots and weights of every formula U_j^i, which occurs in (13), are available or can be computed with cost proportional to n_i.

If we first generate all vectors $\mathbf{i} \in \mathbb{N}^d$ with $q-d+1 \leq |\mathbf{i}| \leq q$ and then compute the knots and weights of all cubature formulas

$$(-1)^{q-|\mathbf{i}|} \cdot \binom{d-1}{q-|\mathbf{i}|} \cdot (U_1^{i_1} \otimes \cdots \otimes U_d^{i_d})$$

then we get a bound

$$\operatorname{cost}(q,d) \leq L \cdot d \cdot \tilde{n}(q,d) \tag{20}$$

uniformly in q and d. Here L is a small positive constant that does not dependent on the choice of the sequence $(n_i)_i$ and sequences of quadrature formulas U_j^i.

Assume that the sets $X_j^1, X_j^2, \ldots$ are pairwise disjoint for every j. Then $n(q,d) = \tilde{n}(q,d)$ and therefore

$$\operatorname{cost}(q,d) \leq L \cdot d \cdot n(q,d).$$

See Remarks 4 and 8 for further discussion.

Let $(n_i)_i$ be given and assume that (17) and (18) hold. For fixed $k \in \mathbb{N}$, Lemma 2 and (20) imply

$$\operatorname{cost}(k+d,d) \preceq L \cdot (3/2)^k \cdot d \cdot n(k+d,d)$$

as d tends to infinity. We may omit the factor $(3/2)^k$ if $X_j^1 \not\subset X_j^2$ for every j.

Definition. Let sequences of quadrature formulas U_j^i be given and consider the corresponding cubature formulas $A(q,d)$. Let $\ell, d \in \mathbb{N}$ and choose the minimal q such that $A(q,d)$ has degree ℓ of exactness. Define

$$N(\ell,d) = n(q,d).$$

Corollary 2. *Assume* (11) *as well as* (17) *and* (18). *Then* $A(k+d,d)$ *has (at least) a degree* $2k+1$ *of exactness and uses*

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

knots. Here k *is fixed and* d *tends to infinity.*

Remark 2. The lower bound (9) yields

$$N_{\min}(2k+1,d) \ge \binom{k+d}{d} \approx \frac{1}{k!} \cdot d^k.$$

We conclude that the polynomial dependence on d in Corollary 2 is optimal. The lower bound $\binom{k+d}{d}$ can be improved, see Möller (1979), but optimal constants in estimates of the form

$$N_{\min}(2k+1,d) \approx c_k \cdot d^k$$

seem to be unknown.

The upper bound (8) is only of order

$$N_{\min}(2k+1,d) \le \binom{2k+1+d}{d} \approx \frac{1}{(2k+1)!} \cdot d^{2k+1}.$$

Remark 3. So far we have studied exactness of $A(q,d)$ under very weak assumptions on the quadrature formulas U_j^i. For asymptotic results with fixed d and q tending to infinity as well as for error bounds the following properties are useful:

(i) $X_j^{i-1} \subset X_j^i$ for every i and j.

(ii) The sequence n_i is "slowly" growing.

(iii) $\sup_{i,j} \|U_j^i\| < \infty$.

We also want to have:

(iv) The formulas U_j^i are easy to construct.

In fact, for standard weight functions such formulas may simply be copied from the literature.

By (i) we get embedded formulas $A(q,d)$, which are based on sparse grids

$$H(q,d) = \bigcup_{|\mathbf{i}|=q} X_1^{i_1} \times \cdots \times X_d^{i_d}. \tag{21}$$

Hence the number of points in $H(q,d)$ is reduced, cf. (19). By (ii) we get a slowly growing sequence $n(q,d)$. Property (iii) is not directly related to polynomial exactness. Still it is important since it leads to error bounds and reasonable stability of the formulas $A(q,d)$, see Remarks 6 and 9. Stability is further improved by (i), since weights of different sign at common points partially cancel.

At this point we mention that (iii) implies

$$\|A(q,d)\| \leq \sum_{s=q-d+1}^{q} \binom{s-1}{d-1} \cdot \binom{d-1}{q-s} \cdot \left(\sup_{i,j} \|U_j^i\|\right)^d \leq c_{d,\varrho} \cdot q^{d-1} \tag{22}$$

with a positive constant $c_{d,\varrho}$.

Assuming (i) we obtain a simple recursion for $n(q,d)$. Let $q \geq d$ as well as $X_j^0 = \emptyset$ and $n_0 = 0$. By (21),

$$\begin{aligned} H(q+1,d+1) &= \bigcup_{s=1}^{q-d+1} \bigcup_{|\mathbf{i}|=q+1-s} X_1^{i_1} \times \cdots \times X_d^{i_d} \times (X_{d+1}^s \setminus X_{d+1}^{s-1}) \\ &= \bigcup_{s=1}^{q-d+1} H(q+1-s,d) \times (X_{d+1}^s \setminus X_{d+1}^{s-1}). \end{aligned}$$

Thus

$$n(q+1,d+1) = \sum_{s=1}^{q-d+1} n(q+1-s,d) \cdot (n_s - n_{s-1}). \tag{23}$$

4. Symmetric Weight Functions on Bounded Domains

In this section we assume that Ω is a bounded hyperrectangle in $\mathbb{R}^d$. Without loss of generality we consider

$$\Omega = [-1,1]^d.$$

Furthermore we assume that ϱ is a product of symmetric weight functions ϱ_j, i.e.,

$$\varrho_j(-x) = \varrho_j(x) \tag{24}$$

for $x \in [-1,1]$ and every j.

We will use symmetric quadrature formulas U_j^i with odd numbers n_i of knots. Hence we even have a degree

$$m_i = n_i$$

of exactness, cf. (12). As previously we use X_j^i to denote the knots of the formula U_j^i.

Properties (i)–(iv) from Remark 3 hold for certain quadrature formulas that were already studied in Novak and Ritter (1996, 1997). Namely, take interpolatory quadrature formulas

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

where

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

and $x_1^1 = 0$. Hence U_j^i uses Chebyshev knots of the second kind together with the endpoints of the interval $[-1,1]$. The same sparse grid $H(q,d)$ is studied also in Sprengel (1997).

In order to satisfy (i) and (ii) with n_i as small as possible we take

$$n_1 = 1 \qquad \text{and} \qquad n_i = 2^{i-1} + 1 \tag{25}$$

for $i > 1$. Hence we have (11) for $m_i = n_i$ as well as (12). Furthermore, (17) and (18) hold, and we can apply the results from Section 3 to the resulting cubature formulas $A(q, d)$.

Lemma 3 (Schmitt (1997), Satz 8). *For every $q \geq d$,*

$$\widetilde{n}(q, d) \leq (2^d - 1) \cdot n(q, d).$$

Proof. As the statement obviously holds for $d = 1$, we assume $d \geq 2$. Put

$$\widehat{n}(q, d) = \sum_{|\mathbf{i}|=q} n_{i_1} \dots n_{i_d}.$$

Inductively, using (23), we obtain

$$n(q + 1, d) \geq 2 \cdot n(q, d)$$

for every $q \geq d$ and

$$\widehat{n}(q, d) \leq 2^{d-1} \cdot n(q, d).$$

By

$$\widetilde{n}(q, d) = \sum_{s=q-d+1}^{q} \widehat{n}(s, d) = n(q, d) \cdot \sum_{s=0}^{d-1} \frac{n(q - s, d)}{n(q, d)} \cdot \frac{\widehat{n}(q - s, d)}{n(q - s, d)} \leq (2^d - 1) \cdot n(q, d)$$

the statement follows. □

Remark 4. The simplicity of computing the knots and weights of $A(k+d, d)$ for fixed k and large d has already been demonstrated in Remark 1. For arbitrary d and q Lemma 3 and (20) imply

$$\mathrm{cost}(q, d) \leq L \cdot d \cdot (2^d - 1) \cdot n(q, d).$$

The construction from Remark 1 yields a list of $\widetilde{n}(q, d)$ knots and weights to describe the formula $A(q, d)$. One can easily modify the construction to obtain the minimal list of length $n(q, d)$ within the above cost bound.

The constant $2^d - 1$ in Lemma 3 is far too large for reasonable values of $n(q, d)$, if d is large. For instance, if $n(q, d) \leq 10^9$ and $d \geq 6$, then $2^d - 1$ may be replaced by 60. The last bound was found by extensive computations.

We do not have to solve any nonlinear equation to construct $A(q, d)$, since the knots of U^i_j and $A(q, d)$ are given explicitly. To obtain the correct weights in the univariate case one has to solve a linear system of equations. In some cases one also can copy the weights from the literature, of course. For $\varrho_j = 1$ explicit formulas for the respective a^i_j are known, see Gentleman (1972) and Brass (1977).

From Theorem 1 we get the following result.

Corollary 3. *Let $q = \sigma d + \tau$ with $\sigma \in \mathbb{N}$ and $\tau \in \{0, \ldots, d-1\}$. Then $A(q,d)$ has degree of exactness*

$$\ell(q,d) = \begin{cases} 2(q-d)+1 & \text{if } q < 4d \\ 2^{\sigma-2} \cdot (d+1+\tau) + 2d - 1 & \text{otherwise.} \end{cases}$$

In the following table we give some explicit values for $N(\ell, d)$ in dimensions $d = 5$, 10, 15, 20, and 25.

TABLE 1

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$
3	11	21	31	41	51
5	61	221	481	841	1 301
7	241	1 581	5 021	11 561	22 201
9	801	8 801	40 001	120 401	286 001
11	2 433	41 265	261 497	1 018 129	2 976 161
13	6 993	171 425	1 471 297	7 314 609	26 139 361
15	*19 313*	652 065	7 367 857	46 106 289	199 876 961
17	*51 713*	2 320 385	33 647 617	261 163 009	1 361 884 161

The table consists of numbers $n(q,d)$ with minimal q such that $\ell(q,d) \geq \ell$. We have used the recursion (23) to compute $n(q,d)$.

For fixed $\ell = 2k+1$ and large d the asymptotic behavior of $N(\ell,d)$ is determined in Corollary 2 and further discussed in Remark 2. Now we study the dual situation where d is fixed and ℓ tends to infinity.

Lemma 4 (Müller-Gronbach (1997), Lemma 1)**.** *For $q \to \infty$ and fixed d*

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

Corollary 4. *For $k \to \infty$ and fixed d*

$$N(2k+1,d) \leq c_d \cdot k^d \cdot (\log k)^{d-1}$$

with a positive constant c_d.

Proof. Take $q = \sigma d$ with

$$\sigma = 3 + \lceil \log_2((k-d+1)/(d+1)) \rceil$$

and apply Corollary 3 and Lemma 4. □

Remark 5. The upper bound (8) reads

$$N_{\min}(2k+1,d) \le \binom{2k+1+d}{d} \approx \frac{2^d}{d!} \cdot k^d$$

for fixed d. The upper bound from Corollary 4 is slightly worse. However, in Table 1 we have $\binom{2k+1+d}{d} \le N(2k+1,d)$ only for $l = 15, 17$ and $d = 5$. The respective numbers are slanted.

Remark 6. If $\varrho_j = 1$ then U_j^i is a classical Clenshaw-Curtis formula, which has only positive weights. For arbitrary weight functions ϱ_j the formula U_j^i may have negative weights. However, if there is a $p > 1$ such that $\varrho_j \in L_p$ for all j, then (iii) holds. See Sloan and Smith (1978).

By (iii) and (25) we get

$$\|A(q,d)\| \le c_{d,\varrho} \cdot (\log n)^{d-1}, \tag{26}$$

for all d and q, see Novak and Ritter (1997). Here $c_{d,\varrho}$ is a positive number that only depends on d and ϱ. Estimates of the form (26) are important to prove error bounds.

It turns out that the resulting cubature formulas $A(q,d)$ are universal, i.e, they are almost optimal (up to logarithmic factors) for many different function classes. Specifically, we have the error bound (6) for all standard smoothness classes

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

with $r, d \in \mathbb{N}$, see Novak and Ritter (1997). Here $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$ is used to denote a partial derivative of order $|\boldsymbol{\alpha}| = \alpha_1 + \dots + \alpha_d$. For all nonisotropic spaces

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

with $r, d \in \mathbb{N}$ we have the error bound (7), see Novak and Ritter (1996). Here $\boldsymbol{\alpha} \le r$ means $\alpha_i \le r$ for every $i = 1, \dots, d$.

Remark 7. The interior points that are used by U_j^i are the zeros of the orthogonal polynomials for the weight function

$$\varrho_j(x) = (1 - x^2)^{1/2}.$$

Therefore a slight modification of the above construction leads to some improvement for this particular weight function. Namely, take

$$n_i = 2^i - 1$$

and

$$x_j^i = -\cos \frac{\pi j}{n_i + 1}$$

where $j = 1, \dots, n_i$. Then

$$m_i = 2^{i+1} - 3,$$

and Theorem 1 implies

$$\ell(q,d) = 2^{\sigma} \cdot (d+1+\tau) - 2d - 1$$

for $q = \sigma d + \tau$ with $\sigma \in \mathbb{N}$ and $\tau \in \{0,\dots,d-1\}$. In some cases we get an essential improvement. For instance, $N(17,5) = 18943$ with the above modification while we had $N(17,5) = 51713$ previously. However, the asymptotic statements in Corollaries 2 and 4 cannot be improved.

5. General Weight Functions

We consider integrals over arbitrary hyperrectangles $\Omega \subset \mathbb{R}^d$ with arbitrary weight functions ϱ of tensor product form.

We use Gaussian formulas U_j^i for the weight ϱ_j. Let X_j^i denote the set of knots that are used by U_j^i. We choose

$$n_i = 2^{i-1}$$

as the cardinality of X_j^i. Clearly this yields a degree

$$m_i = 2^i - 1$$

of exactness. Therefore (11), (12), (17), and (18) are satisfied. Moreover, properties (ii) and (iii) hold, while (i) does not hold. Thus we can apply the results from Section 3.

Remark 8. The cost of computing $A(k+d,d)$ with fixed k and large d is of order $L \cdot d \cdot n(k+d,d)$, see Remark 1.

Similar to the proof of Lemma 3 one can show that $\tilde{n}(q,d) \le c_{d,\varrho} \cdot n(q,d)$ in the present case. Therefore, by (20),

$$\operatorname{cost}(q,d) \le L \cdot d \cdot c_{d,\varrho} \cdot n(q,d).$$

Note that $c_{d,\varrho} = 1$ for $\varrho = 1$.

Gaussian formulas can be taken from the literature or can be efficiently computed, see, e.g., Gautschi (1979) and Ehrich (1993).

Theorem 1 yields the following fact.

Corollary 5. *Let $q = \sigma d + \tau$ with $\sigma \in \mathbb{N}$ and $\tau \in \{0,\dots,d-1\}$. Then $A(q,d)$ has degree of exactness*

$$\ell(q,d) = \begin{cases} 2(q-d)+1 & \text{if } q < 3d \\ 2^{\sigma-1} \cdot (d+1+\tau) - 1 & \text{otherwise.} \end{cases}$$

Now we study the number $n(q,d)$ of knots in the cubature formula $A(q,d)$. Recall that $n(q,d) \le \tilde{n}(q,d)$.

Lemma 5. *For every $q \ge d$,*

$$\tilde{n}(q,d) = \sum_{p=q-d+1}^{q} \binom{p-1}{d-1} \cdot 2^{p-d}.$$

Proof. The statement follows from

$$\#(X_1^{i_1} \times \cdots \times X_d^{i_d}) = 2^{|\mathbf{i}|-d}$$

and (19). □

In Table 2 we give explicit upper bounds for $N(\ell, d)$, which are based on Corollary 5 and on the estimate from Lemma 5. For $\ell > 3$ all numbers in Table 1 are less than the respective ones in Table 2.

TABLE 2

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$
3	11	21	31	41	51
5	71	241	511	881	1 351
7	351	2 001	5 951	13 201	24 751
9	1 471	13 441	54 911	154 881	352 351
11	*5 502*	77 505	427 007	1 515 009	4 152 511
13	*18 932*	397 825	2 907 647	12 849 409	42 154 111
15	*61 112*	1 862 145	17 791 487	97 047 809	378 739 711
17	*187 552*	8 085 505	99 652 607	665 387 009	3 071 424 511

By Lemma 5,

$$n(q, d) \leq c_d \cdot 2^q \cdot q^{d-1}.$$

Analogously to Corollary 4 we obtain the following result.

Corollary 6. *For $k \to \infty$ and fixed d*

$$N(2k+1, d) \leq c_d \cdot k^d \cdot (\log k)^{d-1}$$

with a positive constant c_d.

Hence the observations from Remark 5 also apply in the general case. In the range of Table 2 the Tchakalov bound is superior for $d = 5$ and $\ell = 11, \ldots, 17$. The respective numbers are slanted.

Remark 9. Observe that $n(q, d) \geq 2^{q-d}$. Together with (22) this implies (26). It is well known that this bound and the polynomial exactness of $A(q, d)$ lead to error bounds for various function classes. Furthermore, general estimates for the Smolyak construction are available for tensor product problems. See, e.g., Wasilkowski and Woźniakowski (1995) and Novak and Ritter (1996, 1997).

In particular, if Ω is bounded then the error bounds from Remark 6 hold.

6. Symmetric Weight Functions

In this section we assume the symmetry (24) for every univariate weight function ϱ_j as in Section 4. However, we drop the boundedness assumption for Ω. We improve the upper bound from Corollaries 4 and 6. As a drawback of the following approach we do not have good error bounds.

We study symmetric formulas with properties (i), (ii), and (iv), while (iii) may not hold. We take

$$n_i = m_i = 2i - 1$$

for every $i \in \mathbb{N}$ and arbitrary symmetric sets $X_j^1 \subset X_j^2 \subset \dots$ with $\# X_j^i = n_i$. The sequence $(n_i)_i$ is as small as possible, and the conditions (11), (12), (17), and (18) are satisfied. In order to obtain small values $\|U_j^i\|$ the knots must be chosen appropriately.

We can apply the results from Section 3. In particular, Theorem 1 reads as follows.

Corollary 7. *Let $q \geq d$. Then $A(q,d)$ has degree of exactness*

$$\ell(q,d) = 2(q-d) + 1.$$

Remark 10. In the special case where, in addition to (24),

$$\varrho_1 = \dots = \varrho_d$$

it is possible to take

$$U_1^i = \dots = U_d^i. \tag{27}$$

In this case the resulting formulas $A(q,d)$ are fully symmetric. This means that $x \in H(q,d)$ implies

$$(\pm x_{p(1)}, \dots, \pm x_{p(d)}) \in H(q,d)$$

for each permutation p of $\{1, \dots, d\}$ and arbitrary signs. The weights coincide for all these knots.

Genz (1986) studied a construction of fully symmetric formulas that is based on a sequence of nonnegative and pairwise different real numbers λ_i with $\lambda_0 = 0$. The numbers λ_i are called generators and they uniquely determine a d-dimensional cubature formula $G(q,d)$ of degree $2(q-d)+1$ of exactness for every d and $q \geq d$. We have

$$A(q,d) = G(q,d)$$

if

$$X^{i+1} \setminus X^i = \{\pm \lambda_i\},$$

where X^i is the set of knots that is used by the quadrature formula (27).

The number $n(q,d)$ can further be reduced by choosing special sets X^i of knots such that certain of the weights (and knots) of $A(q,d)$ disappear. See Genz (1986) for the weight $\varrho_j = 1$ on $\Omega_j = [-1,1]$ and Genz and Keister (1996) for the weight $\varrho_j(x) = \exp(-x^2)$ on $\Omega_j = \mathbb{R}$. We have already discussed respective results in the introduction.

Remark 11. A nonclassical polynomial space $E(q,d)$ of exactness for general $A(q,d)$ is presented in Lemma 1. For the method of this section the spaces $\mathbb{P}(\ell(q,d),d)$ and $E(q,d)$ are rather close. We have

$$\mathbb{P}(2(q-d)+1,d) \subset E(q,d) \subset \mathbb{P}(2q-d,d).$$

In contrast,

$$\mathbb{P}(\ell(q,d),d) \subset E(q,d) \subset \mathbb{P}(2^{q-d}+d,d)$$

for the method from Section 4 if $q > d$, and

$$\mathbb{P}(\ell(q,d),d) \subset E(q,d) \subset \mathbb{P}(2^{q-d+1}+d-2,d)$$

for the method from Section 5. The above inclusions cannot be improved. Observe that

$$\frac{2^{q-d}}{\ell(q,d)} \asymp 2^{q(1-1/d)}$$

for the methods from Sections 4 and 5.

There is a simple recursion for the number $n(q,d)$ of knots that is used by $A(q,d)$.

Lemma 6. *We have*

$$n(q+1,d+1) = n(q,d+1) + n(q,d) + n(q-1,d)$$

for $q \geq d$ and $n(q,1) = 2q-1$.

Proof. By (23),

$$n(q+1,d+1) = 2 \cdot \sum_{s=1}^{q-d+1} n(q+1-s,d) - n(q,d).$$

Now the recursion easily follows. □

As in the previous sections we give some explicit values for $N(\ell,d)$ in dimensions $d = 5$, 10, 15, 20, and 25. Table 3 consists of numbers $n(q,d)$ with minimal q such that $\ell(q,d) \geq \ell$. For $\ell > 5$ all numbers in Table 3 are less than the respective ones in Table 1. They are also smaller than the upper bound (8), see Remark 12.

For fixed dimension and large degree of exactness we have the following estimate.

Corollary 8. *If d is fixed and $k \to \infty$ then*

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

Proof. Put $g(k,0) = 1$ and

$$g(k,d) = n(k+d,d)$$

for $d \in \mathbb{N}$ and $k \in \mathbb{N}_0$. By Lemma 6,

$$g(k+1,d+1) = g(k,d+1) + g(k+1,d) + g(k,d) \tag{28}$$

for $k,d \in \mathbb{N}_0$. Hence g is symmetric and Lemma 2 yields the asymptotic behavior of $n(k+d,d)$ for fixed d. By Corollary 1, $N(2k+1,d) \leq n(k+d,d)$. □

TABLE 3

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$
3	11	21	31	41	51
5	61	221	481	841	1 301
7	231	1 561	4 991	11 521	22 151
9	681	8 361	39 041	118 721	283 401
11	1 683	36 365	246 047	982 729	2 908 411
13	3 653	134 245	1 303 777	6 814 249	24 957 661
15	7 183	433 905	5 984 767	40 754 369	184 327 311
17	13 073	1 256 465	24 331 777	214 828 609	1 196 924 561

We derive an explicit formula for $n(k+d,d)$.

Theorem 2. *For every $k \in \mathbb{N}_0$ and $d \in \mathbb{N}$ we have*

$$N(2k+1,d) \le n(k+d,d) = \sum_{s=0}^{\min(k,d)} \binom{k}{s} \cdot \binom{k+d-s}{k}.$$

Proof. We use the function g, as defined in the proof of Corollary 8. Define generating functions

$$h_k(x) = \sum_{d=0}^{\infty} g(k,d) \cdot x^d.$$

Then (28) implies

$$h_k(x) = h_{k-1}(x) + x \cdot h_k(x) + x \cdot h_{k-1}(x)$$

for $k \ge 1$. Furthermore

$$h_0(x) = \sum_{d=0}^{\infty} x^d = \frac{1}{1-x}.$$

Therefore

$$h_k(x) = \frac{(1+x)^k}{(1-x)^{k+1}} = \sum_{s=0}^{k} \binom{k}{s} x^s \cdot \sum_{r=0}^{\infty} \binom{k+r}{r} x^r.$$

Hereby the explicit formula for $n(k+d,d) = g(k,d)$ follows. The upper bound for $N(2k+1,d)$ follows from Corollary 1. $\square$

Remark 12. Theorem 2 immediately implies

$$N(2k+1,d) \le \binom{k+d}{d} \cdot \min(2^k, 2^d). \tag{29}$$

Here the binomial coefficient is the lower bound (9), and the right-hand side in (29) is asymptotically sharp for fixed d and $k \to \infty$ and vice versa.

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

$$N(2k+1,d) \le n(k+d,d) < \binom{2k+1+d}{d}. \tag{30}$$

Here the right-hand side is the upper bound (8). A proof of (30) uses induction on d and k. In particular one uses Lemma 6 to obtain

$$\begin{aligned} n(k+d+2,d+1) &= n(k+d+1,d+1) + n(k+d+1,d) + n(k+d,d) \\ &< \binom{2k+d+2}{d+1} + \binom{2k+d+3}{d} + \binom{2k+d+1}{d} \\ &< \binom{2k+d+2}{d+1} + \binom{2k+d+3}{d} + \binom{2k+d+2}{d} \\ &= \binom{2k+d+4}{d+1}. \end{aligned}$$

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