Cubature Formulas for Symmetric Measures in Higher Dimensions with Few Points

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Abstract

We study cubature formulas for d-dimensional integrals with an arbitrary symmetric weight function of product form. We present a construction that yields a high polynomial exactness: for fixed degree $\ell = 5$ or $\ell = 7$ and large dimension d the number of knots is only slightly larger than the lower bound of Möller and much smaller compared to the known constructions.

We also show, for any odd degree $\ell = 2k+1$, that the minimal number of points is almost independent of the weight function. This is also true for the integration over the (Euclidean) sphere.

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1 Introduction

Let us start with a special case of our results: We find cubature formulas with

$$N(5,d,1) = d^2 + 7d + 1, \quad \text{and} \quad N(7,d,1) = (d^3 + 21d^2 + 20d + 3)/3$$

points such that the integral

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

is exactly computed for all polynomials of degree at most 5 or 7, respectively. This improves the known cubature formulas for degree 5 and $d \geq 8$ and for degree 7 with $d \geq 10$. The lower bound of Möller (1979) takes the form

$$(1) \quad N_{\min}(5,d,1) \geq d^2 + d + 1 \quad \text{and} \quad N_{\min}(7,d,1) \geq (d^3 + 3d^2 + 8d)/3.$$

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Hence, for our method, we obtain

$$N(5,d,1) \approx N_{\min}(5,d,1) \qquad \text{and} \qquad N(7,d,1) \approx N_{\min}(7,d,1). \tag{2}$$

We use $\approx$ to denote the strong equivalence of sequences, i.e.,

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

The best results (for large d) from the literature, see Stroud (1971) and the online tables of Cools, see Cools (2003), are given by

$$N_{\mathrm{old}}(5,d,1) = 2d^2 + 1 \qquad \text{and} \qquad N_{\mathrm{old}}(7,d,1) = (4d^3 - 6d^2 + 14d + 3)/3. \tag{3}$$

More generally, we study cubature formulas

$$Q_n(f) = \sum_{i=1}^{n} a_i\, f(\mathbf{x}_i), \qquad a_i \in \mathbb{R},\ \mathbf{x}_i \in \Omega, \tag{4}$$

for d-dimensional integrals

$$I_d^{\varrho}(f) = \int_{\Omega} f(\mathbf{x})\, \varrho(\mathbf{x})\, d\mathbf{x}. \tag{5}$$

Concerning the integral we always assume

$$\Omega = \Omega_1 \times \cdots \times \Omega_d$$

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

$$\varrho(\mathbf{x}) = \varrho_1(x_1) \ldots \varrho_d(x_d)$$

of the weight function ϱ. We assume that the ϱ_i are symmetric,

$$\varrho_i(x) = \varrho_i(-x)$$

with $\varrho_i \geq 0$ and integrability of all polynomials, although these assumptions can be relaxed. Some of our results can be slightly improved in the fully symmetric case where, in addition, all the ϱ_i coincide.

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

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

We define

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

to be the minimal number n of knots needed by any cubature formula Q_n of degree ℓ of exactness.

The numbers $N_{\min}(\ell, d, \varrho)$ and corresponding cubature formulas are only known in exceptional cases, see, e.g., Schmid (1983), Berens, Schmid, Xu (1995), and Cools (1997). Thus one is interested in upper and lower bounds for this quantity.

One is often interested in cubature formulas with knots inside the domain and positive weights. While $\mathbf{x}_i \in \Omega$ can always be satisfied by our method, we usually have positive and negative weights. Actually we request $\mathbf{x}_i \in \Omega$, see (4), although the lower of Möller also holds without this assumption.

2 Problem, Main Results, and Conjecture

The lower bound of Möller (1979) for centrally symmetric weight functions is the following: If k is odd then

$$N_{\min}(2k+1,d,\varrho) \geq 2\dim \mathbb{P}_e(k,d) = \binom{d+k}{d} + \sum_{s=1}^{d-1} 2^{s-d}\binom{s+k}{s}.$$

If k is even then

$$N_{\min}(2k+1,d,\varrho) \geq 2\dim \mathbb{P}_o(k,d) - 1 = \binom{d+k}{d} + \sum_{s=1}^{d-1}(1-2^{s-d})\binom{s+k-1}{s}.$$

Here $\mathbb{P}_e(k,d)$ denotes the subspace of $\mathbb{P}(k,d)$ generated by even polynomials and $\mathbb{P}_o(k,d)$ is the subspace generated by odd polynomials. We obtain (1) as special cases and for large d the lower bounds are of the order

$$\approx \frac{2d^k}{k!}.$$

See the book Mysovskikh (1981) or Cools (1997) and, for the explicit formula, Lu, Darmofal (2004).

The best upper bounds were of the form

$$\approx \frac{2^k\, d^k}{k!}. \tag{6}$$

They can be proved with "fully symmetric formulas" (if the ϱ_i are equal) or (in the general case) with the "Smolyak method" or with "sparse grids". All these notions are very much related, see Section 3. Even for special weight functions ϱ and/or for special $\ell = 2k+1$ better bounds were not known. Hence there is a gap between the lower and the upper bound of a factor of 2^{k-1} and we only knew (before we wrote this paper) of one exception: For the weight function

$$\varrho(\mathbf{x}) = \exp(-\|\mathbf{x}\|_2^2), \tag{7}$$

it is known for $\ell = 5$ that

$$d^2 + 3d + 3 \tag{8}$$

function values are enough, see Lu, Darmofal (2004).

Observe that the weight function (7) is invariant with respect to rotations. Hence one might ask whether a result similar to (8) holds for all symmetric weight functions. We conjecture that

$$N_{\min}(2k+1,d,\varrho) \approx \frac{2d^k}{k!} \tag{9}$$

holds for all ϱ and all k, hence the Möller bound is almost optimal. In this paper we prove this conjecture for $k=2$ and $k=3$, see Theorem 1 for more details. We also prove that the numbers $N_{\min}(2k+1,d,\varrho)$ only mildly depend on the weight function ϱ, see Theorem 2 for the details.

3 Some facts about the Smolyak method

We study a special case of the Smolyak method, as we need it in the following. We also present methods with the upper bound (6), since they are used (twice) for our new algorithm with the improved bound. We believe that this proof technique can be used to establish the conjecture (9) in full generality. Everything in this section is known or a minor modification of known results, see Novak, Ritter (1999).

We construct cubature formulas to compute the integral (5) as follows. First we select 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 properties: The formula U_j^i is exact for all univariate polynomials of degree m_i, where

$$m_i \geq 2i - 1. \tag{10}$$

The formula U_j^i uses the knots X_j^i, the number $n_i = |X_j^i|$ of knots satisfies

$$n_i \leq 2i - 1. \tag{11}$$

We also assume that the X_j^i are symmetric and "embedded" or "nested", i.e.,

$$X_j^{i-1} \subset X_j^i \qquad \text{for every } i \text{ and } j. \tag{12}$$

By (10) and (11) the weights of U_j^i are uniquely determined by its knots. Formulas with this property are often 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 $|\mathbf{i}| = i_1 + \cdots + i_d$.

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

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

we use

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

to denote the cardinality of $H(q,d)$.[1] In particular we have $n(q,1)=n_q$ and we put $n(0,1)=n_0=0$. The recursion formula

$$n(q+1,d+1)=\sum_{s=1}^{q-d+1} n(q+1-s,d)\cdot(n_s-n_{s-1}) \tag{14}$$

for $n(q,d)$ is known, see Novak, Ritter (1999).

Remark 1. 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 also

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

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 fully symmetric formulas from Genz (1986) and Genz and Keister (1996) are of the Smolyak form (13). Numerical integration with the Smolyak construction was already studied in Smolyak (1963). There are many other papers on the Smolyak method. The papers Gerstner, Griebel (1998), Novak, Ritter (1999), and Petras (2003) study the polynomial exactness of $A(q,d)$. See also Novak, Ritter, Schmitt, Steinbauer (1999) and the recent survey on sparse grids by Bungartz, Griebel (2004).

The following result is well known, see Corollary 1 of Novak, Ritter (1999).

Lemma 1. *Assume* (10). *Then $A(d+k,d)$ has (at least) a degree $\ell=2k+1$ of exactness.*

Now we present formulas for the number $n(q,d)$ of knots that are used by $A(q,d)$. We consider two cases, important for the following.

The case $n_i=2i-1$.

Using (14) one obtains the recursion

$$n(q+1,d+1)=n(q,d+1)+n(q,d)+n(q-1,d) \tag{15}$$

for $q\ge d$ and $n(q,1)=2q-1$ and $n(d,d)=1$. Table 1 consists of numbers $n(q,d)$ with minimal q such that $n(q,d)\ge\ell$, these numbers are called $N(\ell,d)$.

Using (15) one can get an explicit formula for $n(k+d,d)$, see Novak, Ritter (1999).

[1] Observe that some elements of the sparse grid might get a zero weight in the formula $A(q,d)$. This would decrease the number of needed function values. Hence the "actual" number of needed function values for $A(q,d)$ might be smaller than $n(q,d)$.

Table 1: Number of knots for Smolyak's method with $n_i = 2i - 1$

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	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

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

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

Remark 2. Lemma 2 immediately implies

$$n(k+d,d) \le \binom{k+d}{d} \cdot \min(2^k, 2^d). \tag{16}$$

The case $n_i = 2i - 1$ for $i \neq 3$ and $n_3 = 3$.

If we take the Gaussian formulas U_j^2 with 3 knots for ϱ_j, then we already have exactness 5 and so we can take $U_j^3 = U_j^2$ and still have (10). Altogether we have

$$n_i = 2i - 1 \quad \text{for} \quad i \neq 3, \quad n_3 = 3. \tag{17}$$

Observe that in this case the sets X_j^2 are determined by the weights ϱ_j, we cannot choose these sets. All the other sets X_j^i can be chosen arbitrarily for $i > 2$, but we still assume (12). Similarly as (15) we now obtain from (14) the recursion

$$\begin{aligned} n(q+2,d+1) \;&=\; n(q+1,d+1) + n(q+1,d) + n(q,d) \\ &\quad -2n(q-1,d) + 4n(q-2,d) - 2n(q-3,d). \end{aligned}$$

With this simple modification we obtain the values of Table 2.

Remark 3. Later the following will be important for the two versions of Smolyak's algorithm: In the case $n_i = 2i - 1$ we can take arbitrary symmetric sets X_j^i, in particular we can take

$$X_1^2 = \cdots = X_d^2.$$

Table 2: Number of knots for method (17)

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$
3	11	21	31	41	51
5	51	201	451	801	1 251
7	151	1 201	4 151	10 001	19 751
9	401	5 301	27 701	90 601	227 001
11	1 003	19 505	146 507	643 009	2 040 011
13	2 133	63 805	655 017	3 775 769	15 056 061
15	4 223	188 745	2 584 167	19 111 089	94 680 111
17	8 113	511 625	9 224 937	85 920 449	522 028 561

We also can normalize the weights ϱ_j in such a way that the U_j^2 have the form

$$U_j^2(f) = \gamma f(-x) + \beta_j f(0) + \gamma f(x),$$

where γ (and x) do not depend on j. In addition, we can choose the X_j^i in such a way that $\|\mathbf{x}\|_2 \le \alpha$ for each $\mathbf{x} \in H(q,d)$, where α is the (given) radius of the domain Ω of integration. This means that each rotation maps $\mathbf{x}$ to a point in Ω.

In the second case, however, we have to use the 3 Gauß-knots for $X_j^2 = X_j^3$.

Remark 4. Later we project the points $H(q,d)$ of $A(q,d)$ to a sphere of fixed radius. The origin is not projected. This projection reduces the number of points, the number of projected points $n^*(d+k,d)$ also depends on the sets X_j^i. We only need the second case, where $n_i = 2i-1$ for $i \ne 3$ and $n_3 = 3$. In the case $k=2$ and $k=3$ one obtains

$$n(d+2,d) = 2d^2+1 \quad \text{and} \quad n^*(d+2,d) = 2d^2$$

and

$$n(d+3,d) = (4d^3 - 6d^2 + 20d + 3)/3 \quad \text{and} \quad n^*(d+3,d) = (4d^3 - 6d^2 + 8d)/3.$$

For the last formula observe that $H(d+3,d)$ contains 7 points of the form $\mathbf{x} = (\alpha, 0, \ldots, 0)$ that are projected onto two different points, hence

$$n(d+3,d) = n^*(d+3,d) + 4d + 1.$$

It seems to be difficult to compute the smallest possible number $n^*(d+k,d)$ for general k, but it is clear that

$$n(d+k,d) \ge n^*(d+k,d) \ge 2^k \binom{d}{k}.$$

Hence, for large d, we have $n(d+k,d) \approx n^*(d+k,d)$.

4 Known results for the Lebesgue measure

Here we explain the best known upper bounds for $N_{\min}(\ell, d, 1)$ that we found in the literature. Again we only discuss results for large d.[2]

The results for $\ell \in \{3,5,7\}$ are classical results that can be found in Stroud (1971):

$n = 2d$ for the degree $\ell = 3$; this bound is sharp, $N_{\min}(3, d, \varrho) = 2d$;

$n = 2d^2 + 1$ for the degree $\ell = 5$;

$n = (4d^3 - 6d^2 + 14d + 3)/3$ for the degree $\ell = 7$.

These results can be obtained with Smolyak's method, we explain the case $\ell = 7$: First we take, as in (17), the values $n_2 = n_3 = 3$ and $n_4 = 7$. Now observe that the 4 new points of X_j^4 are symmetric but otherwise arbitrary. Hence we can take (together with 0) the 5-point Gauß rule with degree 9. This means that $2d$ weights disappear and hence n is decreased by $2d$ compared to the general situation of (17).

The best results (so far) for $\ell > 7$ can be described in the following way: We use again the sequence $m_i \geq 2i - 1$ and so called "delayed Kronrod-Patterson-formulas". The n_i are defined as follows: $n_1 = 1$, $n_2 = n_3 = 3$, $n_4 = n_5 = n_6 = 7$, $n_7 = \cdots = n_{12} = 15$, $n_{13} = \cdots = n_{24} = 31$ and so on. Some of these numbers are larger than $2i - 1$ and hence we can modify those n_i, used by Petras (2003), to

$$\tilde{n}_i := \min(n_i, 2i - 1).$$

In this way one obtains the values from Table 3, see Genz (1986) who obtained the same results.

Table 3: Known values for the Lebesgue measure

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$
3	10	20	30	40	50
5	51	201	451	801	1 251
7	141	1 181	4 121	9 961	19 701
9	391	5 281	27 671	90 561	226 951
11	903	19 105	145 607	641 409	2 037 511
13	1 733	60 205	642 417	3 745 369	14 996 061
15	3 263	168 825	2 473 287	18 743 249	93 755 311
17	5 983	431 265	8 522 247	82 703 329	511 676 911

[2] We illustrate this by an example. In the case $d = 10$ and $\ell = 13$ we will mention a method of Genz (1986) using $n = 60\,205$ function values. In the same paper Genz presents another method using only $n = 37\,389$. This method, however, uses more than 2^d points for general d and hence is not good for "large" d.

Remark 5. Observe that, up to now, there is nothing better known than the fully symmetric formulas that were introduced more than 40 years ago. We do not claim that the results of Table 3 are optimal for fully symmetric (or Smolyak) rules. It was proved by Petras (2003), however, that only minor improvements are possible if one uses Smolyak formulas. The same also holds for the more general fully symmetric formulas. For fixed $\ell = 2k+1$ and large d, the number of points is (at least) of the order

$$N(2k+1, d, \varrho) \approx \frac{2^k\, d^k}{k!}, \tag{18}$$

while the lower bound of Möller is only of the order $\frac{2d^k}{k!}$. Observe that (18) holds for all the versions of Smolyak's method that we presented here.

Remark 6. By Lemma 2 we have the bound

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

for the Smolyak methods described here. For fixed k also Kuperberg (2004) obtains a bound of the form

$$N(2k+1, d, 1) \le \binom{k+d}{d} \cdot C_k.$$

The constant C_k is of the order $2 \cdot k^k \cdot k!$, much bigger than 2^k. However, Kuperberg (2004) obtains cubature formulas with positive (even equal) weights. This is a great advantage, in particular if the function values $f(\mathbf{x}_i)$ are given only approximately.

For a cubature formula Q_n we define its condition number

$$\sigma(Q_n) = \frac{\|Q_n\|_\infty}{\|I_d^\varrho\|_\infty} = \frac{\sum_{i=1}^n |a_i|}{\int_\Omega \varrho(\mathbf{x}) d\mathbf{x}}.$$

A cubature formula with positive weights has condition number $\sigma(Q_n) = 1$ if it is exact for the constant functions. The known Smolyak formulas of degree 5 and 7 have a condition number of roughly d^2 and d^3, respectively. See Remark 8 which also shows that our new formulas have roughly the same condition numbers.

5 Cubature formulas for the sphere and for $M_{d,k}$

In the following we need some known results for cubature formulas for the sphere. We use these results and the Smolyak method to construct efficient cubature formulas for the linear functional

$$M_{d,k}(f) = \sum_{\mathbf{x} \in F(d,k)} f(\mathbf{x})$$

where

$$\mathbf{x} \in F(d,k) \quad \Longleftrightarrow \quad x_i \in \{\pm 1, 0\}, \quad \sum x_i^2 = k.$$

Of course $M_{d,k}$ itself is a cubature formula using $2^k\binom{d}{k}$ function values, where $k \le d$. The point is to find a cubature formula for $M_{d,k}$ that is exact for polynomials from $\mathbb{P}(2k+1, d)$ and uses only about $2\binom{d}{k} \approx 2d^k/k!$ points, which is the order of the lower bound of Möller.

To achieve this we use two cubature formulas for the sphere that are exact for polynomials in $\mathbb{P}(2k+1, d)$. The first formula is obtained from the Smolyak method for the Gaussian weight function (7) by projection onto the sphere of radius $\sqrt{k}$. It has the form

$$w\, M_{d,k}(f) + Q_r(f) \tag{19}$$

where $Q_r(f)$ is a cubature formula with $r = O(d^{k-1})$ points and $w > 0$. In particular, we can take $r \le n^*(d+k, d) - 2^k\binom{d}{k}$ with $n^*(d+k, d)$ from Remark 4. This leads to

$$r \le 2d \quad \text{for} \quad k = 2 \qquad \text{and} \qquad r \le 2d^2 \quad \text{for} \quad k = 3.$$

This works for any degree $2k+1$ of exactness. The second formula $\widetilde{Q}_n(f)$ for $k = 2, 3$ is taken from Mysovskikh (1968), see also Mysovskikh (1981). It uses

$$n = d^2 + 3d + 2 \quad \text{points if} \quad k = 2 \quad \text{and} \quad d \ge 4$$

and

$$n = (d^3 + 9d^2 + 14d + 6)/3 \quad \text{points if} \quad k = 3 \quad \text{and} \quad d \ge 6.$$

It follows that the formula $w^{-1}(\widetilde{Q}_n(f) - Q_r(f))$ is a cubature formula for $M_{d,k}$ exact for polynomials from $\mathbb{P}(2k+1, d)$ which uses at most

$$d^2 + 5d + 2 \qquad \text{and} \qquad (d^3 + 15d^2 + 14d + 6)/3 \tag{20}$$

points for $k = 2$ and $k = 3$, respectively.

Let us finally explain how a Smolyak formula for the Gaussian weight function leads via projection onto the sphere $R\,\mathbb{S}^{d-1}$ of radius $R = \sqrt{k}$ to a cubature formula of the same degree of exactness. To this end, for $r > 0$, let ω_r be the surface measure on the sphere of radius r. Let also P be the radial projection from $\mathbb{R}^d \setminus \{0\}$ onto $R\,\mathbb{S}^{d-1}$ given by $P\mathbf{x} = R\mathbf{x}/\|\mathbf{x}\|_2^2$. Furthermore, let

$$Q_n(f) = \sum_{i=1}^{n} a_i f(\mathbf{x}_i)$$

be an arbitrary cubature formula which is centrally symmetric. Obviously, any Smolyak formula considered above has this property. We assume that Q_n has degree of exactness $2k+1$ for the Gaussian weight function. Let $\mathbf{x}^\alpha = x_1^{\alpha_1} \ldots x_d^{\alpha_d}$ be a monomial of degree $|\alpha| = \alpha_1 + \ldots + \alpha_d = 2k$. Using polar coordinates, we obtain

$$\begin{aligned}
\int_{\mathbb{R}^d} \mathbf{x}^\alpha \exp(-\|\mathbf{x}\|_2^2) d\mathbf{x} &= \int_0^\infty \int_{r\,\mathbb{S}^{d-1}} \mathbf{x}^\alpha d\omega_r(\mathbf{x}) e^{-r^2} dr \\
&= \int_0^\infty (r/R)^{d-1+2k} e^{-r^2} dr \int_{R\,\mathbb{S}^{d-1}} \mathbf{x}^\alpha d\omega_R(\mathbf{x}) \\
&= c(R, d, k) \int_{R\,\mathbb{S}^{d-1}} \mathbf{x}^\alpha d\omega_R(\mathbf{x}).
\end{aligned}$$

We also have

$$Q_n(\mathbf{x}^\alpha) = \sum_{i=1}^{n} a_i \mathbf{x}_i^\alpha = \sum_{i=1}^{n} a_i (\|\mathbf{x}_i\|_2/R)^{2k} (P\mathbf{x}_i)^\alpha.$$

Whenever one of the points $\mathbf{x}_i = 0$, we simply drop the corresponding term. Since

$$Q_n(\mathbf{x}^\alpha) = \int_{\mathbb{R}^d} \mathbf{x}^\alpha \exp(-\|\mathbf{x}\|_2^2) d\mathbf{x},$$

we obtain that

$$PQ_n(\mathbf{x}^\alpha) = \int_{R\mathbb{S}^{d-1}} \mathbf{x}^\alpha d\omega_R(\mathbf{x})$$

where

$$PQ_n(f) = \sum_{i=1}^{n} b_i f(P\mathbf{x}_i)$$

with

$$b_i = \frac{a_i \|\mathbf{x}_i\|_2^{2k}}{R^{2k} c(R, d, k)}.$$

So $PQ_n(f)$ is a cubature formula for the sphere $R\mathbb{S}^{d-1}$ which is exact for homogeneous polynomials of degree $2k$. Since it inherits the central symmetry from Q_n, it is also exact for homogeneous polynomials of degree $2k+1$. Since any polynomial in $\mathbb{P}(2k+1, d)$ restricted to $R\mathbb{S}^{d-1}$ is a sum of two homogeneous polynomials of degree $2k$ and $2k+1$, respectively, PQ_n is exact for all such polynomials.

If we choose the sets X_j^2 in the construction of the Smolyak formula for the Gaussian measure equal, say $X_j^2 = X^2 = \{-a, 0, a\}$, then the points $\mathbf{x} \in aF(d,k)$ are present in the Smolyak formula and get equal positive weights. So the projection of this formula to the sphere $R\mathbb{S}^{d-1}$ has indeed the form (19).

Remark 7. It will be important later on that the cubature formula derived for $M_{d,k}$ uses only points on the same sphere of radius $R = \sqrt{k}$ where the points in $F(d,k)$ live.

6 Cubature formulas for general weight functions

We now derive our main result which is formulated in the following theorem.

Theorem 1. *Let Ω and ϱ be as always and let $k = 2, 3$. In the case $k = 2$ we assume $d \geq 4$, in the case $k = 3$ we assume $d \geq 6$. Then there exists a cubature formula Q_n for I_d^ϱ with degree $2k+1$ of exactness which uses at most*

(21) $$d^2 + 9d + 1 \qquad \text{and} \qquad (d^3 + 33d^2 + 14d + 3)/3$$

points for $k = 2$ and $k = 3$, respectively. If the one-dimensional weight functions ϱ_i are equal (the fully symmetric case) then the number of points can be reduced to

(22) $$d^2 + 7d + 1 \qquad \text{and} \qquad (d^3 + 21d^2 + 20d + 3)/3$$

for $k = 2$ and $k = 3$, respectively.

Proof. We start by describing how one can pass from the special cubature formulas for $M_{d,k}$ constructed in the preceding section to cubature formulas for general weight functions ϱ as in the introduction. By proper scaling, we may assume that the radius of the domain Ω of integration is at least $\sqrt{k}$. First, choose a Smolyak formula Q_m for ϱ that is exact for polynomials from $\mathbb{P}(2k+1,d)$ and satisfies $X_1^2 = \ldots = X_d^2 = \{-1,0,1\}$. Then Q_m has the form

$$Q_m = vM_{d,k} + Q_s \tag{23}$$

for some $v > 0$ and

$$s = n(k+d,d) - 2^k \binom{d}{k}.$$

In general, we have to use the case where $n_i = 2i-1$ for all $i \geq 1$. Then we obtain

$$s = 4d+1 \qquad \text{and} \qquad s = (18d^2+3)/3$$

for $k = 2$ and $k = 3$, respectively. Now we replace the part $M_{d,k}$ in (23) with the formula derived in the preceding section which uses at most as much points as given in (20). By Remark 7 all points of the final cubature formula

$$\frac{v}{w}(\widetilde{Q}_n - Q_r) + Q_s$$

are in the interior of Ω. This cubature formula needs at most $n+r+s$ function values. This leads to cubature formulas with

$$d^2 + 9d + 3 \qquad \text{and} \qquad (d^3 + 33d^2 + 14d + 9)/3$$

points for $k = 2$ and $k = 3$, respectively, which exceeds (21) by just two knots.

A further reduction is possible if knots of $\widetilde{Q}_n$, Q_r and/or Q_s coincide. We explain how this leads to the reduced number of knots in (22) in the fully symmetric case. The reduction by two knots in the general case is achieved similar (and easier).

To simplify notation, we denote by $M_{d,k}^r$ for $r > 0$ the cubature formula

$$M_{d,k}^r(f) = \sum_{\mathbf{x} \in F^r(d,k)} f(\mathbf{x})$$

where

$$\mathbf{x} \in F^r(d,k) \quad \Longleftrightarrow \quad x_i \in \{\pm r, 0\}, \quad \sum x_i^2 = kr^2.$$

Observe that $M_{d,k}^1 = M_{d,k}$.

We further need some notation for fomulas derived from the simplex. Let S be a regular simplex with vertices in the unit sphere $\mathbb{S}^{d-1}$. Let $S_{d,k}^r$ be the cubature formula

$$S_{d,k}^r(f) = \sum_{\mathbf{x} \in G^r(d,k)} (f(\mathbf{x}) + f(-\mathbf{x}))$$

where $G^r(d,k)$ is the set of all projections of the centers of the $(k-1)$-dimensional faces of S onto the sphere of radius r. For the formulas of degree 7 we need one more cubature formula. Denote by p_{ij} the $(d+1)d$ points of the form

$$p_{ij} = \frac{1}{4}v_i + \frac{3}{4}v_j,$$

where v_i and v_j are different vertices of the simplex. Then let $H^r(d)$ be the set of all $rp_{ij}/\|p_{ij}\|$ and define the cubature formula $\widetilde{S}_d^r$ by

$$\widetilde{S}_d^r(f) = \sum_{\mathbf{x}\in H^r(d)} (f(\mathbf{x}) + f(-\mathbf{x})).$$

Finally, let ω_d be the surface area of $\mathbb{S}^{d-1}$.

So assume now that $\varrho_1 = \ldots = \varrho_d$. We further assume without loss of generality that $\Omega \supset [-1,1]^d$. We treat the degree five and seven cases separately.

Degree five. The projected Smolyak formula with degree of exactness 5 for the sphere $\mathbb{S}^{d-1}$ with $d \geq 3$ needs $2d^2$ points and has the form

$$u_1\, M_{d,1}^1 + u_2\, M_{d,2}^{1/\sqrt{2}} \tag{24}$$

with

$$u_1 = \frac{4-d}{2d(d+2)}\omega_d \qquad \text{and} \qquad u_2 = \frac{1}{d(d+2)}\omega_d.$$

This formula can be found in Stroud (1971) or as formula 11) for the sphere in Mysovskikh (1981).

The second formula with degree of exactness 5 for the sphere $\mathbb{S}^{d-1}$ with $d \geq 4$ needs $(d+1)(d+2)$ points and has the form

$$v_1\, S_{d,1}^1 + v_2\, S_{d,2}^1 \tag{25}$$

with

$$v_1 = \frac{d(7-d)}{2(d+1)^2(d+2)}\omega_d \qquad \text{and} \qquad v_2 = \frac{2(d-1)^2}{d(d+1)^2(d+2)}\omega_d.$$

This formula can be found in Mysovskikh (1968) or as formula 7) for the sphere in Mysovskikh (1981).

Putting (24) and (25) together gives the following formula with degree of exactness 5 for $M_{d,2}^{1/\sqrt{2}}$:

$$\frac{1}{u_2}(v_1 S_{d,1}^1 + v_2\, S_{d,2}^1 - u_1 M_{d,1}^1). \tag{26}$$

We also need a Smolyak type formula for the weight function ϱ with degree of exactness 5 which has the form

$$a_1\, M_{d,2}^{1/\sqrt{2}} + a_2\, M_{d,1}^{1/\sqrt{2}} + a_3\, M_{d,1}^{\gamma} + a_4 Q_0, \tag{27}$$

where $Q_0(f) = f(0)$ and $\gamma \in (0,1) \setminus \{1/\sqrt{2}\}$. The coefficients $a_1, \dots, a_4$ can be derived either from the Smolyak construction or from direct computation using Sobolev's theorem which tells us that our formula has the required degree of exactness if it integrates the polynomials $1, x_1^2, x_1^4, x_1^2 x_2^2$ correctly. This leads to a linear system of 4 equations for $a_1, \dots, a_4$ which has a unique solution. To minimize the number of knots we choose $\gamma = 1$.

Finally, we replace $M_{d,2}^{1/\sqrt{2}}$ in formula (27) with the expression (26). This leads to a formula

$$\alpha_1 \left(S_{d,2}^{1/\sqrt{2}} + \frac{d^2(7-d)}{4(d-1)^2} S_{d,1}^{1/\sqrt{2}} \right) + \alpha_2 M_{d,1}^{1/\sqrt{2}} + \alpha_3 M_{d,1}^{1/2} + \alpha_4 Q_0 \tag{28}$$

which is exact of degree 5 for integration with respect to ϱ with $d \geq 4$. The coefficients $\alpha_1, \dots, \alpha_4$ can be directly derived using the polynomials $1, x_1^2, x_1^4, x_1^2 x_2^2$. Alternatively, they are related to $a_1, \dots, a_4$ via

$$\alpha_1 = \frac{2(d-1)^2}{(d+1)^2} a_1, \quad \alpha_2 = a_3 - \frac{4-d}{2} a_1, \quad \alpha_3 = a_2, \quad \alpha_4 = a_4.$$

Observe that we have chosen our formulas so that the final number of knots is $d^2 + 7d + 3$. This can be further reduced to

$$d^2 + 7d + 1$$

if we choose one of the vertices of the regular simplex S as the unit vector $(1, 0, \dots, 0)$. Observe also that in the case $d = 7$ the number of knots reduces even further.

Degree seven. Let us now derive a formula with degree of exactness 7, i.e., $k = 3$. The projected Smolyak formula with degree of exactness 7 for the sphere $\mathbb{S}^{d-1}$ with $d \geq 3$ needs $(4d^3 - 6d^2 + 8d)/3$ points and has the form

$$u_1 M_{d,1}^1 + u_2 M_{d,2}^{1/\sqrt{2}} + u_3 M_{d,3}^{1/\sqrt{3}}. \tag{29}$$

This formula can be found in Stroud (1971) or as formula 21) for the sphere in Mysovskikh (1981).

The second formula with degree of exactness 7 for the sphere $\mathbb{S}^{d-1}$ with $d \geq 6$ needs $(d^3 + 9d^2 + 14d + 6)/3$ points and has the form

$$v_1 S_{d,1}^1 + v_2 S_{d,2}^1 + v_3 S_{d,3}^1 + v_4 \widetilde{S}_d^1. \tag{30}$$

This formula can be found in Mysovskikh (1968) or as formula 13) for the sphere in Mysovskikh (1981).

Putting (29) and (30) together gives the following formula with degree of exactness 7 for $M_{d,3}^{1/\sqrt{3}}$:

$$\frac{1}{u_3} \left(v_1 S_{d,1}^1 + v_2 S_{d,2}^1 + v_3 S_{d,3}^1 + v_4 \widetilde{S}_d^1 - u_1 M_{d,1}^1 - u_2 M_{d,2}^{1/\sqrt{2}} \right). \tag{31}$$

We also need a Smolyak type formula for the weight function ϱ with degree of exactness 7 which has the form

$$a_1\, M_{d,3}^{1/\sqrt{3}} + a_2\, M_{d,2}^{1/\sqrt{3}} + a_3\, M_{d,1}^{1/\sqrt{3}} + a_4\, M_{d,2}^{\gamma_1} + a_5\, M_{d,1}^{\gamma_1} + a_6\, M_{d,1}^{\gamma_2} + a_7 Q_0, \tag{32}$$

where $Q_0(f) = f(0)$ and the numbers γ_1 and γ_2 and $1/\sqrt{3}$ are pairwise different, between 0 and 1. To minimize the number of knots in the following we choose $\gamma_1 = 1/\sqrt{2}$ and $\gamma_2 = 1$.

Finally, we replace $M_{d,3}^{1/\sqrt{3}}$ in formula (32) with the expression (31). This leads to a formula of the form

$$\alpha_1 \left(v_1\, S_{d,1}^1 + v_2\, S_{d,2}^1 + v_3\, S_{d,3}^1 + v_4\, \widetilde{S}_d^1\right) +$$
$$\alpha_2\, M_{d,1}^1 + \alpha_3\, M_{d,2}^{1/\sqrt{2}} + \alpha_4\, M_{d,1}^{1/\sqrt{2}} + \alpha_5\, M_{d,2}^{1/\sqrt{3}} + \alpha_6\, M_{d,1}^{1/\sqrt{3}} + \alpha_7\, Q_0.$$

The constants $\alpha_1, \ldots, \alpha_7$ can be determined by using the 7 polynomials 1, x_1^2, x_1^4, $x_1^2 x_2^2$, $x_1^2 x_2^2 x_3^2$, $x_1^4 x_2^2$ and x_1^6. Observe that we have chosen our formulas so that the number of knots is

$$(d^3 + 21d^2 + 20d + 9)/3.$$

This can be further reduced to

$$(d^3 + 21d^2 + 20d + 3)/3$$

if we choose one of the vertices of the regular simplex S as the unit vector $(1, 0, \ldots, 0)$. $\square$

Table 4 contains the number of function values for fully symmetric weight functions. Observe that for $\ell = 7$ we have to assume $d \geq 6$.

Table 4: New values for fully symmetric weight functions

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$	$N(\ell,50)$	$N(\ell,100)$
5	61	171	331	541	801	2 851	10 701
7	–	1 101	2 801	5 601	9 751	59 501	404 001

It is interesting to compare these values with the lower bound (1) of Möller, see Table 5.

Table 5: Möller's lower bound

ℓ	$N(\ell,5)$	$N(\ell,10)$	$N(\ell,15)$	$N(\ell,20)$	$N(\ell,25)$	$N(\ell,50)$	$N(\ell,100)$
5	31	111	241	421	651	2 551	10 101
7	80	460	1 390	3 120	5 900	44 300	343 600

Remark 8. For the cube $[-1,1]^d$ with Lebesgue measure, Tables 6 and 7 contain the coefficients a_i and α_i in the cubature formulas (27), (28), (32). The values of $v_1, \ldots, v_4$ and u_1, u_2, u_3 for the degree 7 formula can be found in Mysovskikh (1981).

Table 6: Coefficients for the degree 5 formulas (27) and (28)

i	1	2	3	4
$2^{-d}a_i$	$\frac{1}{9}$	$\frac{22}{45} - \frac{2d}{9}$	$\frac{1}{30}$	$\frac{2d^2}{9} - \frac{37d}{45} + 1$
$2^{-d}\alpha_i$	$\frac{2(d-1)^2}{9(d+1)^2}$	$\frac{d}{18} - \frac{17}{90}$	$\frac{22}{45} - \frac{2d}{9}$	$\frac{2d^2}{9} - \frac{37d}{45} + 1$

Table 7: Coefficients for the degree 7 formula (32)

i	1	2	3	4
$2^{-d}a_i$	$\frac{1}{8}$	$\frac{7}{20} - \frac{d}{4}$	$\frac{23}{70} - \frac{9}{20} + \frac{d^2}{4}$	$\frac{8}{45}$

i	5	6	7
$2^{-d}a_i$	$\frac{32}{63} - \frac{16d}{45}$	$\frac{1}{21}$	$-\frac{d^3}{6} + \frac{5d^2}{9} - \frac{659d}{630} + 1$

Remark 9. Victoir (2004) and Kuperberg (2004) describe, in particular, methods for $\ell = 5$ and positive weights. For $d = 100$ Victoir has $n = 4^{12} = 16\,777\,216$ and this was further improved by Kuperberg to $n = 65\,536$ points with positive weights. See the discussion in Kuperberg (2004).

For general weights the old record was 20 001, see (3). Our method needs 10 701 function values, the lower bound of Möller is 10 101.

7 Independence of the weight function

We now use the Smolyak formulas to show that, for any fixed k, the minimal number of knots needed by a cubature formula of degree $2k+1$ does not essentially depend on the weight function. Since the Möller lower bound is of order d^k, the following theorem shows that the difference can only be in the lower order terms.

Theorem 2. *Let $\Omega^{(j)}$ and $\varrho^{(j)}$, $j = 1, 2$, be two regions and weight functions in $\mathbb{R}^d$ as described in the introduction. For $k = 2, 3, \ldots$, define*

$$c_k = \frac{2^{2k}}{(k-1)!}.$$

Then

$$|N_{\min}(2k+1,d,\varrho^{(1)}) - N_{\min}(2k+1,d,\varrho^{(2)})| \le c_k d^{k-1}$$

for all $d \ge k$.

Proof. Without loss of generality, we assume that the cube $[-1,1]^d$ is contained in the interior of $\Omega^{(1)}$ and $\Omega^{(2)}$. We choose a cubature formula Q_n for $\varrho^{(1)}$ exact for polynomials in $\mathbb{P}(2k+1,d)$ with $n = N_{\min}(2k+1,d,\varrho^{(1)})$. By proper scaling if necessary we may now assume that the knots of Q_n are in the interior of $\Omega^{(2)}$. We also choose, for $j = 1, 2$, Smolyak formulas

$$Q_{m_j}^{Smol} = w_j M_{d,k} + Q_{r_j}$$

for $\varrho^{(j)}$ of degree $2k+1$ with $w_j > 0$. To assure their existence, we have to work with the case $n_i = 2i - 1$ for all i. In this case we can also arrange that the knots of Q_{r_j} are contained in $[-1,1]^d$. Then, for $d \ge k$, the estimate

$$r_j \le 2^k \binom{d+k}{k} - 2^k \binom{d}{k} \tag{33}$$

follows from (16). Now

$$\frac{w_2}{w_1}(Q_n - Q_{r_1}) + Q_{r_2}$$

defines a cubature rule for $\varrho^{(2)}$ exact for polynomials in $\mathbb{P}(2k+1,d)$ with at most $n + r_1 + r_2$ knots. Observe that all the knots used are in the interior of $\Omega^{(2)}$. By (33), to prove the theorem it is enough to verify the elementary inequality

$$2^k \binom{d+k}{k} - 2^k \binom{d}{k} \le \frac{2^{2k}}{(k-1)!} d^{k-1}$$

for $d \ge k$, which is equivalent to

$$(d+k)(d+k-1)\dots(d+1) - d(d-1)\dots(d-k+1) \le k\, 2^k\, d^{k-1}.$$

Since the left-hand side of this inequality does not exceed $(d+k)^k - (d-k)^k$, this is an immediate consequence of

$$(d+k)^k - (d-k)^k = 2 \sum_{\substack{0 \le i \le k \\ i \text{ odd}}} \binom{k}{i} d^{k-i} k^i \le 2 d^{k-1} k \sum_{\substack{0 \le i \le k \\ i \text{ odd}}} \binom{k}{i} = k\, 2^k\, d^{k-1}.$$

□

Remark 10. Similarly, it can be shown that

$$|N_{\min}(2k+1,d,\mu_d) - N_{\min}(2k+1,d,\varrho)| \le c_k d^{k-1},$$

where μ_d is the surface measure on the sphere $\mathbb{S}^{d-1}$ and ϱ is a weight function as in Theorem 2.

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