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Integration of Smooth Functions  
with One Singular Point**

*Ronald Cools and Erich Novak*

*Report TW 308, July 2000*



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## Abstract

We consider the problem of numerical integration for multivariate functions with respect to a radial symmetric weight. We prove that suitable spherical product algorithms have the optimal rate of convergence  $n^{-k/d}$  for  $C^k$ -functions. We also study classes of integrands with a singularity that are  $C^k$  outside the origin. Standard algorithms have high cost for such functions, because they require that the function is smooth everywhere. We construct suitably modified spherical product algorithms with optimal rate of convergence  $n^{-k/d}$  also in this case. In the compact case we can use modified spherical product Gauss formulas with a nonalgebraic degree of precision.

**Keywords :** multivariate integration, spherical product algorithms, optimal rate of convergence, integrands with singularity, Gauss formulas, nonalgebraic degree of precision

**AMS(MOS) Classification :** Primary : 65D32 Secondary : 41A25, 41A55

# SPHERICAL PRODUCT ALGORITHMS AND THE INTEGRATION OF SMOOTH FUNCTIONS WITH ONE SINGULAR POINT

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**1. Introduction.** We motivate our results by a simple *example*. Assume that you want to compute the integral

$$I[f_3] = \int_{x \in \mathbb{R}^3, \|x\| \leq 1} f_3(x) dx$$

for  $f_3(x) = (1 + x_1^2) \cdot \exp(\|x\|)$  by a numerical algorithm. One may use the *classical spherical product Gauss formulas* which have the optimal rate  $n^{-k/3}$  of convergence for all  $C^k(\mathbb{R}^3)$  spaces, see Theorem 1. With  $n = 27\,000$  function evaluations, the error of this algorithm on our example is still larger than  $10^{-5}$ . The integrand  $f_3$  is Lipschitz but not a  $C^1$ -function because of the singularity at the origin. Hence the classical algorithm is not very good. We consider this as a significant problem of the classical algorithm because the distance to a singular point (in this case the origin) appears often in integrands.

With our *modified spherical product Gauss formulas* the error is about  $2.6 \cdot 10^{-11}$  with only  $n = 250$  function evaluations. Observe that

$$f_3(x) = \tilde{f}_3(\varphi_1, \varphi_2, r) = ((\cos \varphi_1)^2 (\cos \varphi_2)^2 r^2 + 1) \exp(r),$$

where  $(\varphi_1, \varphi_2, r)$  are spherical coordinates, see § 4. The function  $\tilde{f}_3$  is very smooth and our algorithm behaves excellent for all integrands that are *smooth if written in spherical coordinates*. After this illustration we describe the contents of the paper in a more systematic way.

Let  $C^k(\mathbb{R}^d)$  be the space of  $k$  times continuously differentiable functions on  $\mathbb{R}^d$  with bounded  $k$ th derivatives,

$$\|D^\alpha f\|_\infty \leq 1 \quad \text{for all } \alpha \in \mathbb{N}^d, |\alpha| = k,$$

and let

$$(1) \quad I_d[f] = \int_{\mathbb{R}^d} f(x) \varrho(\|x\|) dx.$$

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By  $\|x\|$  we denote the Euclidean norm in  $\mathbb{R}^d$  and we assume that  $d > 1$ .

We use the following conditions on the weight  $\varrho$ . We assume that  $r \mapsto r^{d-1} \varrho(r)$  is integrable and  $\varrho$  is non-negative. We exclude the trivial case where  $\varrho = 0$  almost everywhere. An essential condition, which was already used by Wasilkowski and Woźniakowski (2000), is

$$(2) \quad \lim_{t \rightarrow \infty} \varrho(t) t^\beta = 0 \quad \text{for a } \beta > k + d.$$

Then  $I_d[f]$  is well defined for all  $f \in C^k(\mathbb{R}^d)$ .

Standard algorithms for numerical integration for the class  $C^k(\mathbb{R}^d)$  are based on interpolation by some kind of polynomials or piecewise polynomials (splines). There are many such algorithms. In §2 we describe the *classical spherical product Gauss formulas* for the computation of  $I_d[f]$ , see also Stroud and Secrest (1966) and Stroud (1971). For this algorithm one has to assume that all polynomials are integrable. This is possibly only a minor disadvantage since this additional assumption is satisfied for many interesting cases. Soon we will see a more serious disadvantage of classical spherical product Gauss formulas, related to error bounds.

We discuss the optimal rate of convergence, or the order of the complexity, for computing  $I_d[f]$  for  $f \in C^k(\mathbb{R}^d)$ . From general results about adaption we know that it is enough to consider algorithms of the form

$$(3) \quad Q_n[f] = \sum_{i=1}^n w_i f(x_i),$$

see Traub, Wasilkowski and Woźniakowski (1988). The (worst case) error of  $Q_n$  is given by

$$e(Q_n) = e(Q_n, C^k(\mathbb{R}^d)) = \sup_{f \in C^k(\mathbb{R}^d)} |I_d[f] - Q_n[f]|.$$

Assume first that  $\varrho$  has compact support and  $r \mapsto r^{d-1} \varrho(r)$  is integrable. Then it is well known that the optimal rate of convergence for the space  $C^k(\mathbb{R}^d)$  is  $n^{-k/d}$ , i.e., for  $n$  sufficiently large

$$\exists c, C \in \mathbb{R} : c \cdot n^{-k/d} \leq \inf_{Q_n} e(Q_n) \leq C \cdot n^{-k/d}.$$

We refer to Novak (1988) for more details on this topic. In this case the classical spherical product Gauss formulas have the optimal rate of convergence, see § 2.

The case of a general  $\varrho$  is more complicated and was studied only recently in Wasilkowski and Woźniakowski (2001). These authors study the condition (2) and prove [under slightly more restrictive conditions] that it implies that the optimal rate is  $n^{-k/d}$ . The classical spherical product Gauss formulas in general do *not* yield, however, the optimal rate. This follows from results of Curbera (1998) who studied the case  $d = k = 1$  with the Gaussian weight  $\varrho(x) = \exp(-x^2)$ . According to what we wrote above, the optimal rate of convergence for this case is  $n^{-1}$ . The Gaussian formulas, however, only yield the rate  $n^{-1/2}$ .

In this paper we use *spherical product algorithms* for the classes  $C^k(\mathbb{R}^d)$ , because these quadrature formulas are easy to construct and to analyze. These algorithms yield the optimal rate  $n^{-k/d}$ , in the general case introduced above. One has to use univariate quadrature formulas with the optimal rate  $n^{-k}$ , see § 3. We know from

Wasilkowski and Woźniakowski (2000) that such univariate formulas exist. In the compact case ( $\varrho$  has compact support) one can always use Gaussian formulas which have the optimal rate of convergence and, in addition, a high degree of polynomial exactness. In the general (noncompact) case it is enough to modify the quadrature formulas for the coordinate  $r$ . We still can use Gaussian formulas for all other coordinates.

In § 4 we consider the case where  $f$  may have a singularity at the origin and is  $k$  times continuously differentiable in all other points. For example,  $f$  could be of the form

$$(4) \quad f(x) = \|x\| + g(x), \quad \text{where } g \in C^k(\mathbb{R}^d).$$

Such a function is not (globally)  $C^k$  but of course we still can apply the classical algorithms. Instead of the rate  $n^{-k/d}$  we only obtain some fixed rate which does not increase with  $k$ . We construct what we call *modified spherical product algorithms* to obtain the optimal rate  $n^{-k/d}$  also for functions of the form (4), as well as for other functions which are in  $C^k$ , *if written in certain spherical coordinates*; see § 4 for the exact definition of the class  $\tilde{C}^k(\mathbb{R}^d)$ . It is important to use coordinates for which  $r$  is nonnegative. Then functions of the form (4) are in  $C^k$  in these coordinates. The classical spherical product algorithms, as explained in § 3, use coordinates where  $r \in \mathbb{R}$  and  $f$  in (4) is *not* differentiable with respect to  $r$ .

To obtain the optimal rate of convergence in the compact case, we can use *modified spherical product Gauss formulas*. These cubature formulas have a *nonalgebraic degree of precision*, they are exact for functions of the form

$$f(x) = p_1(x) + \|x\| \cdot p_2(x),$$

where  $p_1$  is a polynomial of degree  $2\ell - 1$  and  $p_2$  is a polynomial of degree  $2\ell - 2$ . Such cubature formulas were introduced by Cools and Santos-León (2000).

All presented algorithms are some kind of spherical product formulas, constructed from quadrature formulas for univariate functions. For the modified spherical product formulas the integral

$$I[f] = \int_{-\pi}^{\pi} f(\varphi) |\cos \varphi|^{d-2} d\varphi$$

is important: we need a Gauss quadrature formula with  $2\ell$  points which is exact for all trigonometric polynomials of degree  $2\ell - 1$ . We discuss such formulas in § 5.

**2. The Classical Spherical Product Gauss Formulas.** Tensor product algorithms are easy to describe, and also to analyze. For integrals of the form (1) such algorithms are defined via spherical coordinates. There are different ways to define  $d$ -dimensional spherical coordinates. We follow Stroud (1971) and use the definition

$$(5) \quad \begin{aligned} x_1 &= r \cos \varphi_{d-1} \cos \varphi_{d-2} \dots \cos \varphi_2 \cos \varphi_1 \\ x_2 &= r \cos \varphi_{d-1} \cos \varphi_{d-2} \dots \cos \varphi_2 \sin \varphi_1 \\ x_3 &= r \cos \varphi_{d-1} \cos \varphi_{d-2} \dots \sin \varphi_2 \\ &\dots \\ &\dots \\ x_{d-1} &= r \cos \varphi_{d-1} \sin \varphi_{d-2} \\ x_d &= r \sin \varphi_{d-1}. \end{aligned}$$

Now one uses the new coordinates  $\varphi_1, \dots, \varphi_{d-1}, r$  where the  $\varphi_i$  are in the interval  $[-\pi/2, \pi/2]$  and  $r \in \mathbb{R}$ . To express the integral  $I_d[f]$  in spherical coordinates we need the Jacobian which is given by

$$(6) \quad J_d = r^{d-1} (\cos \varphi_{d-1})^{d-2} (\cos \varphi_{d-2})^{d-3} \dots (\cos \varphi_3)^2 \cos \varphi_2.$$

Observe that  $J_d$  is a tensor product and therefore the whole integral  $I_d[f]$  is now expressed as a tensor product of (weighted) univariate integrals. For monomials we obtain

$$(7) \quad \begin{aligned} I_d[x_1^{\alpha_1} \dots x_d^{\alpha_d}] &= \int_{\mathbb{R}^d} x_1^{\alpha_1} \dots x_d^{\alpha_d} \varrho(\|x\|) dx \\ &= \int_{-\pi/2}^{\pi/2} (\cos \varphi_1)^{\beta_1} (\sin \varphi_1)^{\alpha_2} d\varphi_1 \cdot \\ &\quad \int_{-\pi/2}^{\pi/2} (\cos \varphi_2)^{\beta_2} (\sin \varphi_2)^{\alpha_3} (\cos \varphi_2) d\varphi_2 \cdot \\ &\quad \dots \\ &\quad \int_{-\pi/2}^{\pi/2} (\cos \varphi_{d-2})^{\beta_{d-2}} (\sin \varphi_{d-2})^{\alpha_{d-1}} (\cos \varphi_{d-2})^{d-3} d\varphi_{d-2} \cdot \\ &\quad \int_{-\pi/2}^{\pi/2} (\cos \varphi_{d-1})^{\beta_{d-1}} (\sin \varphi_{d-1})^{\alpha_d} (\cos \varphi_{d-1})^{d-2} d\varphi_{d-1} \cdot \\ &\quad \int_{\mathbb{R}} r^{\beta_d} |r|^{d-1} \varrho(|r|) dr, \end{aligned}$$

where  $\beta_i = \alpha_1 + \dots + \alpha_i$ . Now we discuss the univariate formulas needed for these integrals, to obtain a formula of polynomial degree  $2\ell - 1$ .

Most of the univariate integrals in (7) have the form

$$(8) \quad \int_{-\pi/2}^{\pi/2} (\cos \varphi_k)^{k-1} P(\cos \varphi_k, \sin \varphi_k) d\varphi_k, \quad k = 1, \dots, d-1,$$

where  $P(\cos \varphi_k, \sin \varphi_k)$  is a polynomial in  $\cos \varphi_k$  and  $\sin \varphi_k$ . Stroud (1971) proved that it suffices to consider only those polynomials  $P$  that contain only even powers of  $\cos \varphi_k$  if one uses symmetric quadrature formulas. Substituting  $y_k = \sin \varphi_k$ , these integrals become

$$(9) \quad \int_{-1}^1 (1 - y_k^2)^{\frac{k-2}{2}} \tilde{P}(y_k) dy_k,$$

where  $\tilde{P}$  is an algebraic polynomial of degree at most  $2\ell - 1$ . Stroud (1971) proved that if one has a quadrature formula

$$(10) \quad Q[f] = \sum_{i=1}^{\ell} w_{k,i} f(y_{k,i}) \approx \int_{-1}^1 (1 - y_k^2)^{\frac{k-2}{2}} f(y_k) dy_k$$

that is symmetric and exact whenever  $f$  is a polynomial of degree  $\leq 2\ell - 1$ , this is transformed to a quadrature formula for the integral (8) that is exact for the needed

polynomials  $P(\cos \varphi_k, \sin \varphi_k)$ . One can use Gauss-Jacobi quadrature formulas for (10). These formulas use the zeros of the Jacobi polynomials  $P^{\alpha, \beta}$ , with  $\alpha = \beta = \frac{k-2}{2}$ , as quadrature points.

Since  $\varrho(|r|)|r|^{d-1}$  does not change sign, the last integral in (7) can be approximated by a Gaussian quadrature formula with a (non-standard) weight function.

In this way we obtain the *classical spherical product Gauss formulas*  $G_n$ . With  $\ell$  points in each variable we get  $n = \ell^d$  if  $\ell$  is even and  $n = \ell^d - \ell^{d-1} + 1$  if  $\ell$  is odd. The polynomial degree of exactness is  $2\ell - 1$  and all weights are positive. See Stroud (1971) for proofs and more details.

**THEOREM 1.** *Assume that  $\varrho$  has compact support. Then the classical spherical product Gauss formulas  $G_n$  have the optimal rate of convergence for the space  $C^k(\mathbb{R}^d)$ ,*

$$e(G_n, C^k(\mathbb{R}^d)) \asymp n^{-k/d}.$$

*Proof.* It is well known that this rate cannot be improved. See, for example, Novak (1988). We sketch two different proofs of the upper bound for  $G_n$ . The first is very short, but the second proof can be modified for the general case.

First proof. We get the rate  $n^{-k/d}$  even for the approximation problem (in the  $L_\infty$ -norm), if we use polynomials up to some total degree. See, for example, Schumaker (1981). We get the same rate for the integration error because we use quadrature formulas with positive weights.

Second proof. For  $f \in C^k(\mathbb{R}^d)$  we write

$$f(x_1, \dots, x_d) = \tilde{f}(\varphi_1, \dots, \varphi_{d-1}, r),$$

where  $(x_1, \dots, x_d)$  and  $(\varphi_1, \dots, \varphi_{d-1}, r)$  are related by (5). Then we obtain

$$I_d[f] = \int_{-\pi/2}^{\pi/2} \dots \int_{-\pi/2}^{\pi/2} \int_{\mathbb{R}} \tilde{f} \cos \varphi_2 \dots (\cos \varphi_{d-1})^{d-2} |r|^{d-1} \varrho(|r|) dr d\varphi_{d-1} \dots d\varphi_1.$$

If  $f$  is a  $C^k$  function with  $\|D^\alpha f\|_\infty \leq 1$  for all  $|\alpha| \leq k$ , then we also have a bound for all  $\|D^\alpha \tilde{f}\|_\infty$ , for  $|\alpha| \leq k$ . Therefore it is enough to prove error bounds for  $\tilde{f} \in C^k$  and to guarantee that the algorithm is exact for polynomials of degree less than  $k$ .

Observe that this integral is a tensor product of univariate integrals. We want to apply a tensor product algorithm and use a known technique to prove the optimal rate  $n^{-k/d}$  for it. Assume that we have several one-dimensional integrals and that for any of these we have the optimal rate  $n^{-k}$  for certain quadrature formulas. Then one can study the product formulas for the product integral and it turns out that we obtain, using this product formulas, the optimal rate  $n^{-k/d}$  in the multivariate case. See Davis and Rabinowitz (1984, p. 361) and Haber (1970, p. 488–489).  $\square$

We already mentioned in §1 that the Gauss formulas do not always give the optimal rate in the general (non-compact) case. Therefore we study more general spherical product algorithms in § 3. Even in the compact case one may want to modify the classical spherical product Gauss formulas, to deal with functions that have a singularity in the origin. The following examples can serve as a starting point for the modifications in § 4.

**2.1. Examples.** Assume that the integrand has the form

$$(11) \quad f(x) = \tilde{f}(\|x\|)$$

and we also put  $\tilde{f}(-y) = \tilde{f}(y)$ .

In particular we first consider for  $d = 3$  the two examples

$$f_1(x) = \|x\| \quad \text{and} \quad f_2(x) = -\|x\| \log(\|x\|)$$

for the weight function  $\varrho_1 = 1_{[0,1]}$ . Then we obtain

$$(12) \quad G_n[f] = Q_\ell[\tilde{f}],$$

where  $Q_\ell$  is the Gaussian formula with  $n = \ell^d$  points if  $\ell$  is even and  $n = \ell^d - \ell^{d-1} + 1$  if  $\ell$  is odd, for the (univariate) weight function

$$\omega(x) = \frac{1}{2} c_d |x|^{d-1} \varrho(|x|)$$

on  $\mathbb{R}$ . Here  $c_d = 2\pi^{d/2}/\Gamma(d/2)$  is the  $(d-1)$ -dimensional volume of  $\{x : \|x\| = 1\}$ . For  $d = 3$  we have  $c_3 = 4\pi$ .

Even if  $\tilde{f}$  is very smooth on  $\mathbb{R}^+$  then still  $f$  is (in general) only Lipschitz on  $\mathbb{R}$ . Therefore we can not expect a high rate of convergence.<sup>1</sup>

All numerical results in this paper are obtained using Maple V using a sufficiently high precision to guarantee that the rounding errors are small compared to the error of the algorithm. So the errors shown are only due to the algorithm. Observe that all algorithms studied in this paper are stable because we use quadrature formulas with positive weights.

Because of the simple relation (12), one should not compute the integral of a function (11) by means of a product formula. We include these examples only to show that the error of the classical spherical product Gauss formulas is rather large even for some simple functions. We use another test function,

$$f_3(x) = (1 + x_1^2) \cdot \exp(\|x\|),$$

again for the weight function  $\varrho_1 = 1_{[0,1]}$  and  $d = 3$ . Here  $x_1$  refers to the first coordinate of a point  $x$ . In Table 1 we present the absolute errors of the classical spherical product Gauss formulas on our test functions.

TABLE 1  
*Errors of classical spherical product Gauss formulas for  $\varrho_1$ .*

$n$	$f_1$	$f_2$	$f_3$
101	3.53995E-2	7.64671E-2	3.43681E-2
1000	6.02351E-4	1.15635E-3	5.91007E-4
3151	8.02675E-4	2.53171E-3	7.99603E-4
8000	4.81768E-5	1.23438E-4	4.79278E-5
15001	1.19860E-4	4.35621E-4	1.19685E-4
27000	1.04047E-5	3.06692E-5	1.03798E-5
rate	$n^{-1.2}$	$n^{-1.1}$	$n^{-1.2}$

<sup>1</sup>Knut Petras kindly explained us that the theory of Peano kernels could be used to obtain error bounds for functions of the form (11). For us these functions only serve as an example and whenever rates of convergence are mentioned, these are obtained by fitting the numerical results.

We also investigate for  $d = 3$  the above examples with the weight function  $\varrho_2(r) = r^{-2}$  on  $[0, 1]$ . Then we obtain

$$G_n[f] = Q_\ell[\tilde{f}]$$

for functions of the form (11), where  $Q_\ell$  is the Gaussian formula with  $n = \ell^d$  points if  $\ell$  is even and  $n = \ell^d - \ell^{d-1} + 1$  if  $\ell$  is odd, for the constant weight function  $2\pi$  on  $[-1, 1]$ . Using the same functions  $f_i$  from above, with the new weight function on the unit ball of  $\mathbb{R}^3$ , we obtain the numerical results presented in Table 2.

TABLE 2  
*Errors of classical spherical product Gauss formulas for  $\varrho_2$ .*

$n$	$f_1$	$f_2$	$f_3$
101	3.46515E-1	8.70964E-1	3.40221E-1
1000	4.72602E-2	1.17640E-1	4.68792E-2
3151	4.30930E-2	1.54157E-1	4.30033E-2
8000	1.23232E-2	3.90050E-2	1.22977E-2
15001	1.59045E-2	6.48521E-2	1.58924E-2
27000	5.56058E-3	1.98168E-2	5.55540E-3
rate	$n^{-0.6}$	$n^{-0.54}$	$n^{-0.6}$

Finally, we consider  $\varrho_3(r) = \exp(-r^2)$  on  $r \geq 0$ . Of course we cannot apply Theorem 1 to this example, but the classical spherical product Gauss formulas  $G_n$  are still defined.

TABLE 3  
*Errors of classical spherical product Gauss formulas for  $\varrho_3$ .*

$n$	$f_1$	$f_2$	$f_3$
101	4.23539E-1	6.02060E-1	3.76739E-1
1000	2.40454E-2	2.29347E-2	2.10462E-2
3151	5.77879E-2	1.17524E-1	5.57241E-2
8000	6.18114E-3	8.17949E-3	5.80620E-3
15001	2.18175E-2	5.01945E-2	2.13603E-2
27000	2.77470E-3	4.25478E-3	2.66364E-3
rate	$n^{-0.6}$	$n^{-0.5}$	$n^{-0.6}$

If we compare the three weight functions then we can say that  $\varrho_1$  is the simplest weight, the errors converge the quickest. This could be expected, since the weight is bounded and the domain is compact.

For completeness, we summarize in Table 4 the integrands and weight functions that we use in this paper, together with the exact value of the integral. In § 4.1 we will present numerical results for the same test integrals and the modified product algorithm.

**2.2. Discussion.** The classical spherical product Gauss formulas have certain advantages and also disadvantages:

- The algorithm is of product type, hence it is easy to describe and also to analyze.

TABLE 4  
Exact results for test problems

	$\varrho_1 = 1_{[0,1]}$	$\varrho_2 = \ x\ ^{-2} 1_{[0,1]}$	$\varrho_3 = \exp(-\ x\ ^2)$
$f_1(x) = \ x\ $	$\pi$	$2\pi$	$2\pi$
$f_2(x) = -\ x\  \log(\ x\ )$	$\pi/4$	$\pi$	$\pi(\gamma - 1)$
$f_3(x) = (1 + x_1^2) \exp(\ x\ )$	$8\pi(2e - 5)$	$4\pi(4e - 5)/3$	$\frac{61}{24} \pi^{3/2} e^{1/4} (1 + \operatorname{erf}(1/2)) + \frac{23}{12} \pi$

- The rate of convergence is optimal for every  $C^k(\mathbb{R}^d)$  if  $\varrho$  has compact domain.
- The rate of convergence is not optimal for every  $C^k(\mathbb{R}^d)$  in the general case.
- The rate of convergence is poor for functions of the form (4) or (11), even in the compact case.

In § 3 we modify the spherical product Gauss algorithm to obtain the optimal rate of convergence for the space  $C^k(\mathbb{R}^d)$  in the general case. In § 4 we will construct an algorithm of product type with optimal rate, also for general  $\varrho$ , and also for functions of the form (4) or (11).

**3. Spherical Product Algorithms for Smooth Functions.** We use the same coordinates as in § 2, but with optimal algorithms for each variable. We only have to change the quadrature formulas for the variable  $r$ . We obtain an algorithm  $Q_n$  with optimal rate of convergence for the class  $C^k(\mathbb{R}^d)$ , also in the general (non-compact) case. We assume, as always in our paper, that  $r \rightarrow r^{d-1} \varrho(r)$  is integrable with (2).

**THEOREM 2.** *The resulting spherical product algorithm  $Q_n$ , formally defined in the proof, has optimal rate of convergence for the space  $C^k(\mathbb{R}^d)$ ,*

$$e(Q_n, C^k(\mathbb{R}^d)) \asymp n^{-k/d}.$$

*Proof.* We proceed as in the second proof of Theorem 1 and obtain

$$I_d[f] = \int_{-\pi/2}^{\pi/2} \dots \int_{-\pi/2}^{\pi/2} \int_{\mathbb{R}} \tilde{f} \cos \varphi_2 \dots (\cos \varphi_{d-1})^{d-2} |r|^{d-1} \varrho(|r|) dr d\varphi_{d-1} \dots d\varphi_1$$

for  $f \in C^k(\mathbb{R}^d)$ . Again it is enough to prove error bounds for  $\tilde{f} \in C^k$  and to guarantee that the algorithm is exact for polynomials of degree less than  $k$ .

For the variables  $\varphi_1, \dots, \varphi_{d-1}$  we can use the same Gaussian rules as in the classical case, see § 2. Only for the variable  $r$  we need to take another algorithm for the integral

$$I[f] = \int_{\mathbb{R}} f(r) |r|^{d-1} \varrho(|r|) dr$$

which is exact for polynomials of degree less than  $k$  and gives the optimal rate  $n^{-k}$  for  $C^k$ -functions. The existence of such an algorithm follows from known results, if we decompose this integral into

$$I_1[f] = \int_{-R}^R f(r) |r|^{d-1} \varrho(|r|) dr \quad \text{and} \quad I_2[f] = \int_M f(r) |r|^{d-1} \varrho(|r|) dr,$$

where  $M = \{r \in \mathbb{R} \mid |r| > R\}$  and  $R$  is chosen in such a way that  $\varrho$  is bounded on  $M$ . It follows from the known results about the compact case that suitable quadrature formulas exist for  $I_1$ , see Novak (1988). The existence of suitable algorithms for  $I_2$  follows from the results of Wasilkowski and Woźniakowski (2000).  $\square$

**4. Modified Spherical Product Algorithms for Functions with a Singularity.** We already motivated this section in § 2.2. We increase the function classes  $C^k(\mathbb{R}^d)$  and use slightly different coordinates in this section. The  $\varphi_i$  and  $r$  are defined by (5) as in §2 but with

$$(13) \quad r \geq 0, \quad \varphi_{d-1} \in [-\pi, \pi], \quad \text{and} \quad \varphi_i \in [-\pi/2, \pi/2] \quad \text{for} \quad i = 1, \dots, d-2.$$

Again we put

$$f(x_1, \dots, x_d) = \tilde{f}(\varphi_1, \dots, \varphi_{d-1}, r),$$

using these new coordinates. Now we define the larger class  $\tilde{C}^k(\mathbb{R}^d)$  by

$$\tilde{C}^k(\mathbb{R}^d) = C^k(\mathbb{R}^d) \cup \{f \in C(\mathbb{R}^d) \mid \|D^\alpha \tilde{f}\|_\infty \leq 1, \quad |\alpha| \leq k, \quad f \text{ periodic w.r.t. } \varphi_{d-1}\}.$$

This class contains functions which are  $C^k$  “if written in the (new) spherical coordinates”.

One should observe that the algorithms from § 3 are *not* good for functions from  $\tilde{C}^k(\mathbb{R}^d)$ . The reason is that the variable  $r$  takes positive as well as negative values in § 3. Therefore we did not get good error bounds for functions of the form (4) or (11). It is easy, however, to modify the algorithms accordingly.

Again the Jacobian is given by (6). The whole integral  $I_d[f]$  is again expressed as a tensor product of univariate integrals. Most of these integrals are as in the classical case, only the range in two of the integrals differs, and we obtain

$$(14) \quad \begin{aligned} I_d[x_1^{\alpha_1} \cdots x_d^{\alpha_d}] &= \int_{\mathbb{R}^d} x_1^{\alpha_1} \cdots x_d^{\alpha_d} \varrho(\|x\|) dx \\ &= \int_{-\pi/2}^{\pi/2} (\cos \varphi_1)^{\beta_1} (\sin \varphi_1)^{\alpha_2} d\varphi_1 \cdot \\ &\quad \int_{-\pi/2}^{\pi/2} (\cos \varphi_2)^{\beta_2} (\sin \varphi_2)^{\alpha_3} (\cos \varphi_2) d\varphi_2 \cdot \\ &\quad \dots \\ &\quad \int_{-\pi/2}^{\pi/2} (\cos \varphi_{d-2})^{\beta_{d-2}} (\sin \varphi_{d-2})^{\alpha_{d-1}} (\cos \varphi_{d-2})^{d-3} d\varphi_{d-2} \cdot \\ &\quad \int_{-\pi}^{\pi} (\cos \varphi_{d-1})^{\beta_{d-1}} (\sin \varphi_{d-1})^{\alpha_d} |\cos \varphi_{d-1}|^{d-2} d\varphi_{d-1} \cdot \\ &\quad \int_0^\infty r^{\beta_d} r^{d-1} \varrho(r) dr, \end{aligned}$$

where  $\beta_i = \alpha_1 + \dots + \alpha_i$ . Now we discuss the univariate formulas needed for these integrals, to obtain a formula of polynomial degree  $2\ell - 1$ , see also Evans and Swartz (2000, Example 5.5). This algorithm will be exact also for functions of the form

$$(15) \quad f(x) = \|x\| \cdot p(x),$$

where  $p$  is a polynomial of degree (at most)  $2\ell - 2$ . Observe that for  $f$  of the form  $f(x) = \|x\| x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ , the integral  $I_d[f]$  also has the form (14), only  $\beta_d$  has to be increased by one.

We can construct such an algorithm similarly as before. First we assume that  $\varrho$  has compact support. The modifications for the general case are similar as in § 3 and will be discussed later.

The product algorithm has to be exact if all  $\alpha_i$  are even, and the result should be zero when at least one  $\alpha_i$  is odd. For the first  $d - 2$  integrals we use symmetric Gaussian formulas with  $\ell$  points and exactness  $2\ell - 1$ , as in § 2.

Also the last integral is straightforward, we use (for  $\varrho$  with compact support) Gaussian formulas with  $\ell$  points for the weight function  $\omega(x) = x^{d-1} \varrho(x)$  on  $x \geq 0$ . This formula, however, is not symmetric and therefore we need a formula for

$$(16) \quad \int_{-\pi}^{\pi} (\cos \varphi)^\beta (\sin \varphi)^\alpha |\cos \varphi|^{d-2} d\varphi$$

which is exact for all  $\alpha + \beta \leq 2\ell - 1$ . Section 5 is devoted to this integral. At this point we only need to know that the lowest possible number of points for such a quadrature formula is  $2\ell$ , that such a formula always exists and has positive weights.

**THEOREM 3.** *Assume that  $\varrho$  has compact support. Then the resulting algorithm is exact for all functions of the form  $p(x) + \|x\|q(x)$  whenever  $p(x)$  is a polynomial of degree at most  $2\ell - 1$  and  $q(x)$  is a polynomial of degree at most  $2\ell - 2$ . It uses  $2\ell^d$  function evaluations and has positive weights.*

*Proof.* This follows from the construction of the formula.  $\square$

**REMARK 1.** *Let  $R_\ell^d$  be the set of all polynomials of degree  $\ell$  together with functions of the form  $f(x) = \|x\|p(x)$  with a polynomial  $p$  of degree  $\ell - 1$ . Cools and Santos-León (2000) study, among other things, cubature formulas which are exact for  $R_\ell^d$ . They prove that a cubature formula with exactness  $R_{2\ell-1}^d$  must have at least  $\dim(R_{\ell-1}^d)$  points. The dimension of  $R_{\ell-1}^d$  is given by*

$$\dim(R_{\ell-1}^d) = \binom{d+\ell-1}{d} + \binom{d+\ell-2}{d}.$$

For fixed dimension  $d$  and large  $\ell$  we obtain

$$\dim(R_{\ell-1}^d) \approx \frac{2}{d!} \cdot \ell^d,$$

hence the upper bound, given by Theorem 3, is roughly  $d!$  times as large as the lower bound.

**THEOREM 4.** *Assume that  $\varrho$  has compact support. Then the described algorithm has the optimal rate of convergence  $n^{-k/d}$  for the class  $\tilde{C}^k(\mathbb{R}^d)$ .*

*Proof.* The proof is as the proof of Theorem 1 with the difference that now we use the spherical coordinates introduced earlier in this section.  $\square$

For the general (non-compact) case only the algorithm for the variable  $r$  has to be changed. This is done (almost) as in the proof of Theorem 2. For the univariate integral

$$I[f] = \int_0^\infty f(x) x^{d-1} \varrho(x) dx$$

we need quadrature formulas that yield the optimal rate  $n^{-k}$  and are exact for polynomials of degree less than  $k$ .

**THEOREM 5.** *The respective algorithm has the optimal rate  $n^{-k/d}$  for the class  $\tilde{C}^k(\mathbb{R}^d)$ .*

**4.1. Examples.** We will now see how the modified spherical product Gauss formulas behave on the test functions we used in § 2.1. Of course the integrand  $f_1$  now is trivial since the algorithm is designed to produce the exact result for this function.

So we only present numerical results for the test functions  $f_2$  and  $f_3$  for the three weight functions we considered earlier, see Table 4. In Table 5 and 6 we give the absolute errors for these test functions.

TABLE 5  
*Errors of modified spherical product Gauss formulas for  $f_2$ .*

$n$	$\varrho_1$	$\varrho_2$	$\varrho_3$
128	5.97110E-5	8.15778E-3	1.33392E-3
1024	6.45179E-7	6.14338E-4	4.21752E-5
3456	3.73605E-8	1.30222E-4	4.89580E-6
8192	4.61692E-9	4.27581E-5	1.01310E-6
16000	8.83036E-10	1.79180E-5	2.91904E-7
31250	1.64968E-10	7.47693E-6	8.27308E-8
rate	$n^{-2.5}$	$n^{-1.3}$	$n^{-1.9}$

TABLE 6  
*Errors of modified spherical product Gauss formulas for  $f_3$ .*

$n$	$\varrho_1$	$\varrho_2$	$\varrho_3$
128	2.67989E-08	1.36226E-04	8.86155E-04
1024	2.50550E-21	3.05229E-20	1.78478E-11
3456	2.67209E-36	3.53684E-35	2.20710E-20
8192	1.63796E-52	2.26601E-51	5.04496E-30
16000	1.22698E-69	1.74473E-68	3.45789E-40
31250	4.80193E-92	6.98381E-91	1.87378E-53

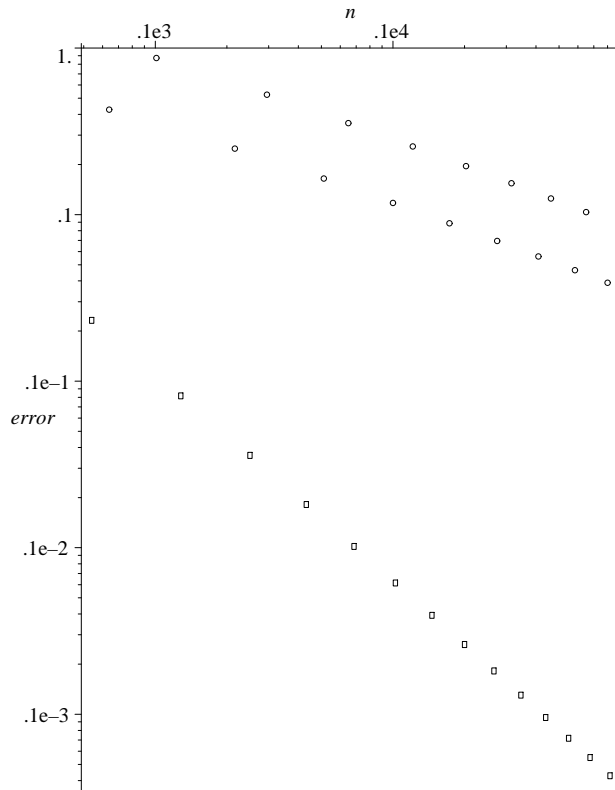
Observe that  $f_2$  is not smooth, even with respect to the new spherical coordinates. Therefore we only get a bounded rate of convergence for this function. Nevertheless, the results are much better than the results of the classical rules. The integrand  $f_3$  is contained in every  $\tilde{C}^k(\mathbb{R}^3)$  and the results are excellent.

In Figures 1 and 2 we show some errors for both the classical and the modified spherical product Gauss formulas on a log-log scale. The circles refer to results of the classical algorithm and the boxes refer to results of the modified algorithm. One clearly sees that for  $f_2$  the convergence is of the form  $n^{-\alpha}$  for some  $\alpha > 0$  and that for  $f_3$  there is an exponential convergence. In all cases the error is significantly smaller for the modified rules than for the classical rules.

**5. Quadrature formulas for  $\int_{-\pi}^{\pi} f(\varphi) |\cos \varphi|^{d-2} d\varphi$ .** In this section we will briefly discuss quadrature formulas for the integral

$$(17) \quad \int_{-\pi}^{\pi} f(\varphi) |\cos \varphi|^{d-2} d\varphi$$

FIG. 1. Error for  $f_2$  and  $\varrho_2$  with classical and modified formulas



which are, for a given  $\ell$ , exact for the class

$$\{(\cos \varphi)^\beta (\sin \varphi)^\alpha \mid 0 \leq \alpha + \beta \leq 2\ell - 1, \alpha, \beta \in \mathbb{N}\}.$$

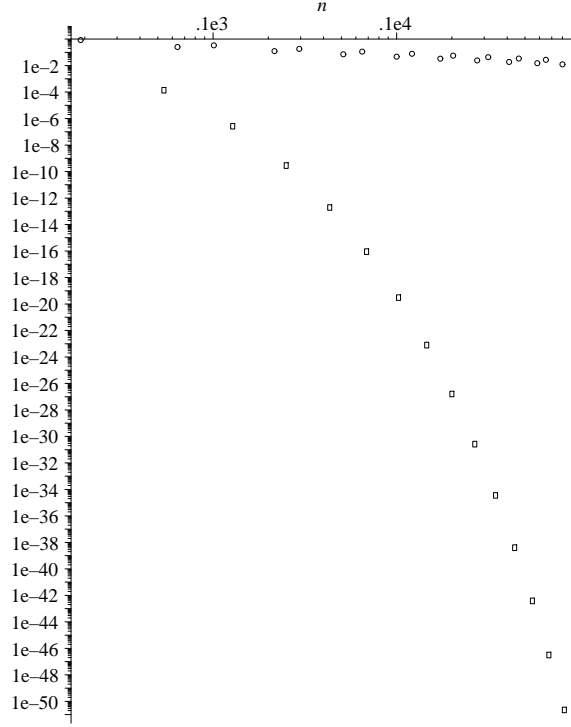
In other words, we are interested in quadrature formulas of trigonometric degree  $2\ell - 1$  for (17). Such quadrature formulas play a crucial role in the modified spherical product rules and we did not encounter them in the literature for  $d \geq 3$ .

In case  $d = 2$  the integral (17) has a constant weight function. It is well known that the minimal number of points in a quadrature formula in this case is  $2\ell$  and that every quadrature formula with equidistant points and equal weights is a minimal quadrature formula. One can shift the points, i.e., there is one free parameter.

Since the weight function  $|\cos \varphi|^{d-2}$  in (17) is nonnegative, it is known that the minimal number of points always is equal to  $2\ell$ . See, e.g., Mysovskikh (1985) and Cools (1997). Furthermore, it is proven by Mysovskikh (1985) that for non-negative weight functions a 1-parameter family of quadrature formulas exists with  $2\ell$  real points in the interval and all weights positive. The proof of Mysovskikh (1985) is constructive. To start this construction the moments

$$\mu_k = \int_{-\pi}^{\pi} e^{-ik\varphi} |\cos \varphi|^{d-2} d\varphi, \quad i^2 = -1, \quad k = 0, \dots, 2\ell - 1$$

FIG. 2. Error for  $f_3$  and  $\varrho_2$  with classical and modified formulas



are required. For even  $d$  one easily obtains

$$\mu_k = \begin{cases} 2^{3-d} \pi \left( \frac{d-2}{\frac{k+d-2}{2}} \right) & \text{for } k \text{ even and } k \leq d \\ 0 & \text{otherwise.} \end{cases}$$

For odd  $d$  one obtains<sup>2</sup>

$$\mu_k = \begin{cases} 2^{3-d} \pi (d-2)! \Gamma\left(\frac{d+k}{2}\right)^{-1} \Gamma\left(\frac{d-k}{2}\right)^{-1} & \text{for } k \text{ even} \\ 0 & \text{for } k \text{ odd.} \end{cases}$$

In our numerical experiments, we always choose the origin as a point of the quadrature formula. Then we obtain a symmetric formula, i.e., if  $x_i$  is a point with corresponding weight  $w_i$ , then  $-x_i$  is also a point with the same weight.

Observe that (17) can be rewritten as

$$\begin{aligned} \int_{-\pi}^{\pi} f(\varphi) |\cos \varphi|^{d-2} d\varphi &= \int_{-\pi/2}^{\pi/2} f(\varphi) (\cos \varphi)^{d-2} d\varphi + (-1)^d \int_{\pi/2}^{3\pi/2} f(\varphi) (\cos \varphi)^{d-2} d\varphi \\ &= \int_{-\pi/2}^{\pi/2} f(\varphi) (\cos \varphi)^{d-2} d\varphi + \int_{-\pi/2}^{\pi/2} f(\varphi + \pi) (\cos \varphi)^{d-2} d\varphi. \end{aligned}$$

<sup>2</sup>We are indebted to Patrick Van gucht whose tedious computations confirmed this.

Each of these integrals has the same form as (8) and can be well approximated by Gauss-Jacobi quadrature formulas, as explained in §2. This also results in a quadrature formula for (17) of degree  $2\ell - 1$  with  $2\ell$  points. In fact, for odd  $\ell$  it coincides with the formula we used in our experiments.

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