ON A RECENT INTERPOLATORY METHOD FOR HIGH DIMENSIONAL INTEGRATION

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Abstract. We discuss numerical integration of smooth functions that are defined on a bounded or unbounded hyperrectangular region. We present numerical results that demonstrate the wide range of applications for our recently invented method. In addition we survey theoretical results. In the symmetric case our method is similar to the fully symmetric rules. However, it also can be used if the weight function is an arbitrary tensor product with different and/or nonsymmetric factors.

1. Introduction

We discuss numerical integration of functions that are defined on a hyperrectangular and possibly unbounded domain $\Omega \subset \mathbb{R}^d$. We focus on functions that have a certain degree of smoothness. We present numerical experiments that demonstrate the wide range of applications for our recently invented method. In addition we survey theoretical results concerning error bounds and polynomial exactness.

In moderate dimensions, say $d \leq 5$, product formulas are a reasonable choice. The corresponding knots form a grid in Ω, and a product formula can easily be implemented if the knots and weights of the one-dimensional rules are at hand. However, due to the exponential growth of the number of knots, product formulas cannot be used in large dimensions.

Among the most popular methods in large dimensions are lattice rules, low discrepancy methods, and Monte Carlo (randomized) methods, see Niederreiter (1992), Sloan and Joe (1994), and Morokoff and Caflish (1995). On the other hand, interpolatory methods seem to be less often used. One major exception is the class of fully symmetric rules for symmetric tensor product weight functions. These formulas were studied by Lyness (1965), McNamee and Stenger (1967), Genz (1986), Cools and Haegemans (1994), Genz and Keister (1996) and other authors. We will demonstrate in this paper that certain interpolatory methods are very competitive even for higher dimensions, say $d = 10$. In the symmetric case our new method is similar to the fully symmetric rules. However, our method can also be used if the weight function is an arbitrary tensor product with different and/or nonsymmetric factors.

Low discrepancy methods and classical Monte Carlo methods do not fully use the smoothness of the integrand. In contrast, our method is almost optimal for different

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classes of smooth functions. This is confirmed by numerical results. For periodic functions suitable lattice rules enjoy similar optimality properties. For most applications, however, one has to deal with the problem of periodization.

2. The Method

Let

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

where $\Omega_\ell \subset \mathbb{R}$ denotes a possibly unbounded interval for $\ell = 1, \ldots, d$. Hence Ω is a hyperrectangular domain in $\mathbb{R}^d$. Furthermore, let

$$\varrho(t) = \varrho_1(t_1) \ldots \varrho_d(t_d)$$

denote a weight function on Ω that is of tensor product form. For simplicity we assume that all d-variate polynomials are integrable with respect to ϱ. We do not require any kind of symmetry for ϱ.

We construct interpolatory cubature formulas to compute the integral

$$I(f) = \int_\Omega f(t) \cdot \varrho(t)\, dt$$

as follows. First we select interpolatory quadrature formulas U_ℓ^i to compute the one-dimensional integrals

$$\int_{\Omega_\ell} f(t) \cdot \varrho_\ell(t)\, dt.$$

These formulas should have the following properties (A), (B), and (C), though in some cases it is also sensible to modify these conditions:

(A) The number m_i of knots that are used by U_ℓ^i is given by

$$m_1 = 1 \qquad \text{and} \qquad m_i = 2^{i-1} + 1$$

for $i > 1$.

(B) The formula U_ℓ^i is exact for all univariate polynomials of degree $m_i - 1$.

(C) The weights are uniformly bounded, i.e.,

$$\sup_{i \in \mathbb{N}} \|U_\ell^i\|_\infty < \infty.$$

Here $\|U_\ell^i\|_\infty$ denotes the sum of the absolute values of the weights of U_ℓ^i.

Due to (B) the weights of U_ℓ^i are uniquely determined by the respective knots. Clearly (C) holds if all formulas U_ℓ^i use positive weights.

A product formula $U_1^{i_1} \otimes \cdots \otimes U_d^{i_d}$ needs $m_{i_1} \ldots m_{i_d}$ 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

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

where $q \geq d$. Here $|\mathbf{i}| = i_1 + \cdots + i_d$. Henceforth we use

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

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

Numerical integration with the Smolyak construction was already studied in Smolyak (1963). Other papers include Baszenski and Delvos (1993), Bonk (1994), Delvos (1990), Genz (1974), Lyness and Sloan (1995), Paskov (1993), Ritter, Wasilkowski, and Woźniakowski (1993), Temlyakov (1992), and Wasilkowski and Woźniakowski (1995). In some of these papers the stress is on the numerical integration of periodic functions.

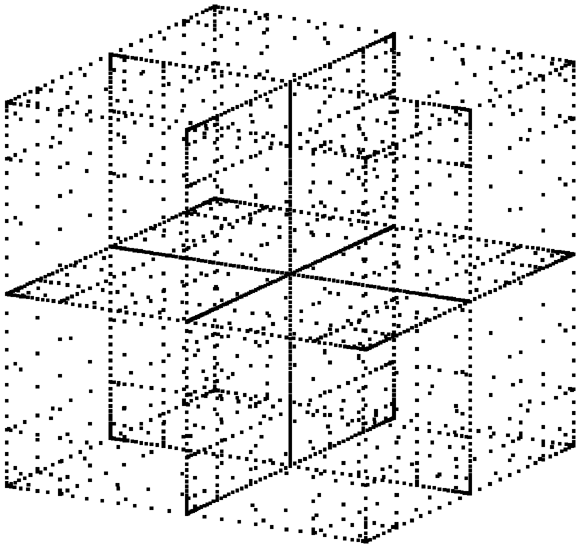
In the fully symmetric case where all weights ϱ_ℓ are identical and symmetric, i.e., $\varrho_\ell(x) = \varrho_\ell(-x)$, it is possible to use the same symmetric formula in each coordinate, in particular we get

$$U^i = U_1^i = \cdots = U_d^i.$$

In this case the resulting $A(q, d)$ is a fully symmetric rule. This choice is often reasonable, but not always. Even in such a symmetric case it can be better to use different U_ℓ^i. If, for example, the integrand is periodic in x_ℓ then it is reasonable to use the simple midpoint rule for this variable. If the integrand only mildly depends on a variable x_ℓ then one may want to change (A) and may want to use different m_i for different coordinates.

Assume that Ω is compact. In this case Novak and Ritter (1996, 1997a) use formulas that are based on Chebyshev knots of the second kind. If $\varrho = 1$ then $U^i = U_\ell^i$ is a classical Clenshaw-Curtis formula. For arbitrary weights ϱ_ℓ we obtain possibly different formulas $U_1^i, \ldots, U_d^i$ all using Chebyshev knots of the second kind. If there is a $p > 1$ such that $\varrho_\ell \in L_p$ for all ℓ then (C) is always true for these knots, see Sloan and Smith (1978).

Chebyshev knots of the second kind lead to imbedded formulas U_ℓ^i and $A(q, d)$ due to (A). This property is important because of several reasons. The number of points that are used by $A(q, d)$ is reduced since different grids have many common points. Furthermore, weights of different sign at common points partially cancel, which leads to better stability properties. Finally, stopping rules can be efficiently implemented, see Section 7. Let us look at the 2561 knots that are used by $A(10, 3)$.



In Sections 5–7 we report on numerical experiments for compact domains Ω and $A(q,d)$ being built of classical Clenshaw-Curtis formulas. In Section 8 we use other univariate formulas as building blocks. Hereby we can deal also with unbounded hyperrectangular domains Ω, and we can adapt our formulas to specific weight functions ϱ. Sometimes we also drop the assumption (A), as already motivated.

3. Basic Properties

We summarize basic properties of $A(q,d)$, which are shown in Novak and Ritter (1996, 1997a). In these papers Chebyshev knots of the second kind are used. The same proofs apply, however, under the more general assumptions (A)–(C).

Let

$$R(q,d)(f) = I(f) - A(q,d)(f)$$

denote the error of $A(q,d)$ for a function f.

1. Assume that Ω is compact. If f has bounded derivatives up to order r on Ω then

$$|R(q,d)(f)| = \mathcal{O}\left(n^{-r/d} \cdot (\log n)^{(d-1)\,(r/d+1)}\right).$$

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

$$|R(q,d)(f)| = \mathcal{O}\left(n^{-r} \cdot (\log n)^{(d-1)\,(r+1)}\right).$$

2. Let V_i denote the space of univariate polynomials of degree $m_i - 1$. Then $A(q,d)$ is exact on

$$\sum_{|\mathbf{i}|=q} (V_{i_1} \otimes \cdots \otimes V_{i_d}).$$

3. The formulas $A(q,d)$ have relatively small weights, since

$$\|A(q,d)\|_\infty = \mathcal{O}((\log n)^{d-1}).$$

Properties 1.) and 2.) show that $A(q,d)$ is universal, i.e., simultaneously optimal up to logarithmic factors, on two different smoothness scales. The first scale is defined by isotropic smoothness conditions, while the second scale involves anisotropic smoothness and is related to partially separable functions. The polynomial exactness of $A(q,d)$ is further investigated in Novak and Ritter (1997b).

Frank and Heinrich (1996) numerically compute the maximal error of $A(q,d)$ on certain function classes and compare it with the error of other methods.

4. The Genz Functions

The testing package of Genz (1984, 1987) is based on a collection of six families of integrands $f_1, \ldots, f_6$ which are defined on $[0,1]^d$. Each of these families is given a name or attribute as follows:

1. OSCILLATORY: $$f_1(t) = \cos\Big(2\pi w_1 + \sum_{i=1}^{d} c_i t_i\Big),$$
2. PRODUCT PEAK: $$f_2(t) = \prod_{i=1}^{d} \left(c_i^{-2} + (t_i - w_i)^2\right)^{-1},$$
3. CORNER PEAK: $$f_3(t) = \Big(1 + \sum_{i=1}^{d} c_i t_i\Big)^{-(d+1)},$$
4. GAUSSIAN: $$f_4(t) = \exp\Big(-\sum_{i=1}^{d} c_i^2 \, (t_i - w_i)^2\Big),$$
5. CONTINUOUS: $$f_5(t) = \exp\Big(-\sum_{i=1}^{d} c_i |t_i - w_i|\Big),$$
6. DISCONTINUOUS: $$f_6(t) = \begin{cases} 0, & \text{if } t_1 > w_1 \text{ or } t_2 > w_2, \\ \exp\left(\sum_{i=1}^{d} c_i t_i\right), & \text{otherwise.} \end{cases}$$

Different test integrals are obtained by varying the parameters $c = (c_1, \ldots, c_d)$ and $w = (w_1, \ldots, w_d)$. The parameter w acts as a shift parameter, and the difficulty of the integrand is monotonically increasing with the $c_i > 0$.

5. A Comparison of Different Methods

Extensive tests are reported in Sloan and Joe (1994) for several cubature formulas in dimension $d = 5$, 8, and 10. The methods ADAPT and COPY usually turned out to be the most successful ones. Here ADAPT denotes an adaptive method that is due to Van Dooren and Ridder (1976) and modified by Genz and Malik (1980). Moreover, COPY denotes an imbedded sequence of lattice rule that is due to Sloan and Joe (1994).

Similar tests for $A(q,d)$, based on the classical Clenshaw-Curtis formulas, are presented in Novak and Ritter (1996). This method is called NEW in that paper and also in the following. It turns out that NEW produces excellent results if the dimension d is relatively large and if the integrand is smooth. If the integrand has only a low degree of smoothness than other methods are superior.

In the following we present results for the test family OSCILLATORY in dimension $d = 10$. These tests were done for the two levels of difficulty ($L = 1$ and $L = 2$) that were proposed by Sloan and Joe (1994). We suggest to further increase the difficulty and define two more levels $L = 3$ and $L = 4$. The four levels of difficulty are defined by

$$\sum_{i=1}^{10} c_i = b_L, \tag{1}$$

where

L	1	2	3	4
b_L	3.15	9.0	20.0	30.0.

Fifty numbers $w \in [0,1]$ and vectors $c' \in [0,1]^d$ are generated independently and uniformly distributed. Then c' is renormalized to satisfy (1). This way we get 50 integrands

$$f(t;L) = \cos\Big(2\pi w + b_L / \sum_{i=1}^{d} c'_i \cdot \sum_{i=1}^{d} c'_i t_i\Big)$$

for each level L of difficulty. The integrals are computed with $A(q,10)$ with $q = 13,\ldots,18$. The corresponding number n of knots is 1581, 8801, 41265, 171425, 652065, and 2320385. For any n we use the median of the actual number

$$-\log_{10} \frac{|I(f) - A(q,d)(f)|}{|I(f)|}$$

of correct digits as the measure for the accuracy. Each of the figures shows the dependence of the median on $\log_{10} n$.

In addition to ADAPT, COPY, and NEW we also use a low-discrepancy method, namely the generalized Faure sequence GF as provided in FINDER. The latter is a software system for computing high dimensional integrals, see Paskov and Traub (1995) and Papageorgiou and Traub (1996). A low-discrepancy sequence is of interest due to the following fact. For every partial derivative of order $|\boldsymbol{\alpha}| = k$ we have

$$f^{(\boldsymbol{\alpha})}(t;L) = f^{(\boldsymbol{\alpha})}(t;1) \cdot b_L^k.$$

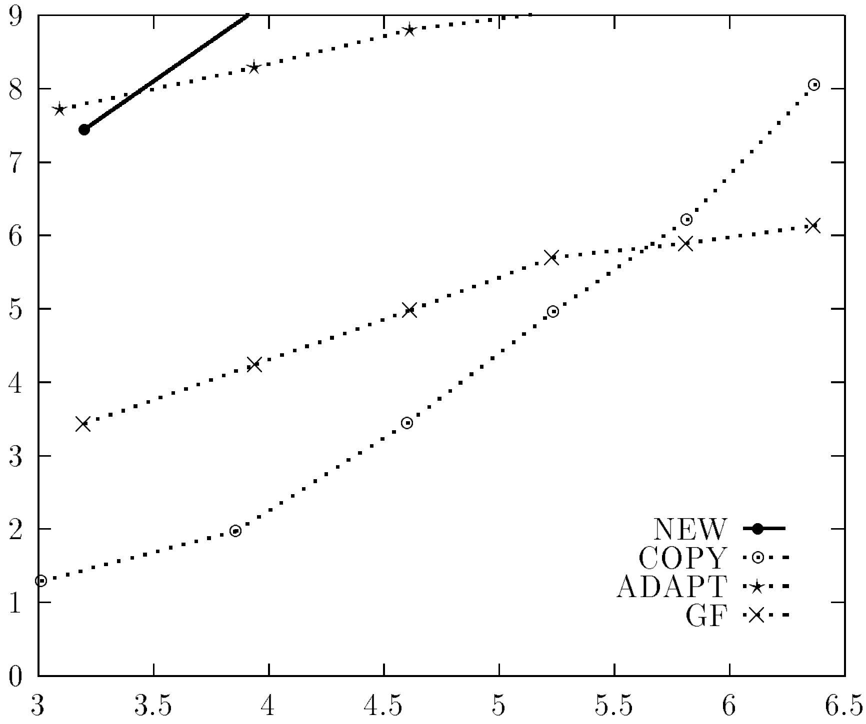
The size of $f^{(1,\ldots,1)}$ is crucial in the error bound for low discrepancy methods. The performance of ADAPT and COPY is also mainly affected by low-order derivatives. In contrast, small derivatives of high order are favorable for NEW, see Section 3. Our results reflect this type of dependence; NEW performs extremely well for small values of b_L but is outperformed for large values.

The results show that there is an extreme difference between the different methods for smooth functions ($L = 1$ and $L = 2$) and a smaller difference for not so smooth functions ($L = 3$ and $L = 4$). Observe that each plot has the same wide range (a factor 10^9) for the error, ranging from 0 to 9 correct digits for $L = 1$, 2 and ranging from -3

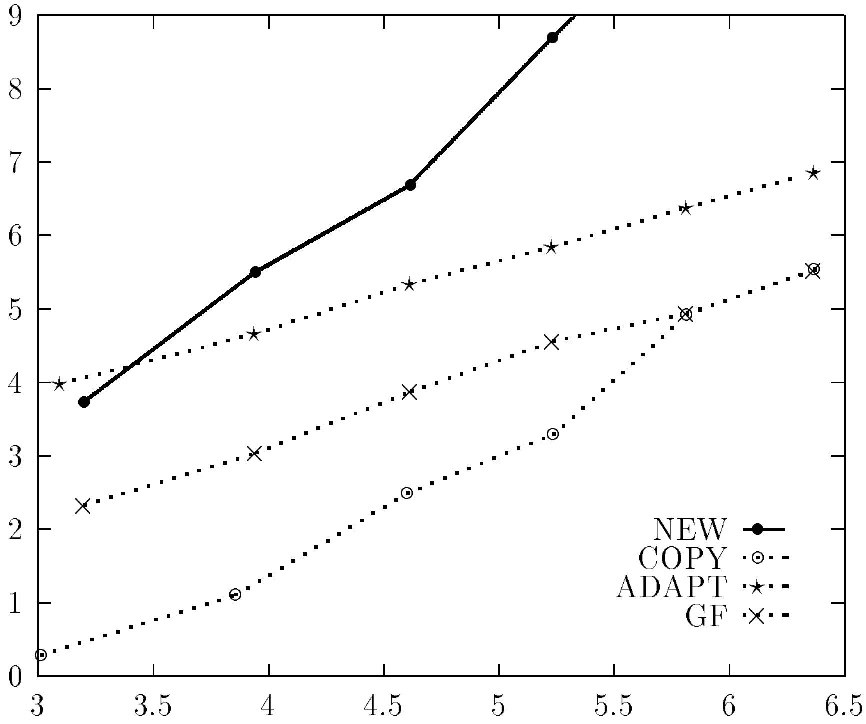
to 6 for $L = 3$, 4. For the smoother functions the actual number of correct digits was sometimes larger than 9. We decided, however, to cut the plots at this limit 9 because for a larger accuracy we had difficulties with rounding: all computations were made in C or C++ and we used the standard data type "double". Therefore also the "correct" values of the integrals are rounded values and we could not decide whether a computed result had 10 or 12 exact digits.

Low discrepancy methods, such as GF, perform well if the integrand has a low smoothness. Interpolatory methods, such as NEW, have a high order of convergence and are therefore superior for large n, say $n \geq n_0$. Observe that n_0 is small for $L = 1$ and 2, while $n_0 \approx 10^4$ for $L = 3$. However, $n_0 \approx 2.3 \cdot 10^6$ for $L = 4$.

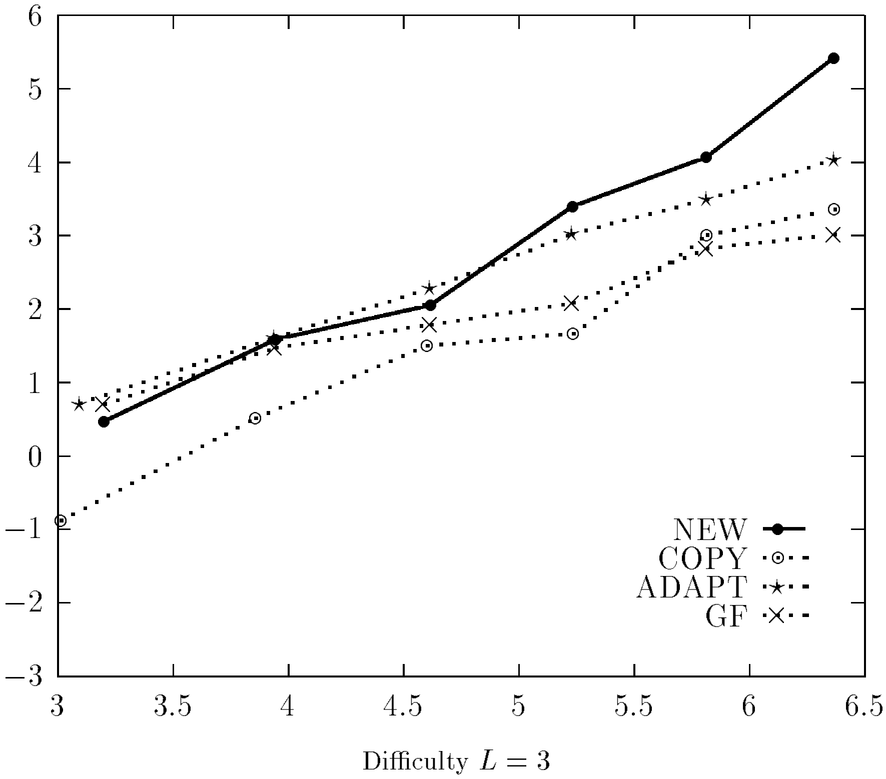
We stress that all results are for dimension $d = 10$ and one cannot expect that the results are similar for other values of d. Some of the methods require an exponential growth of the knots and therefore are useless for $d = 20$ or $d = 50$.



Difficulty $L = 1$



Difficulty $L = 2$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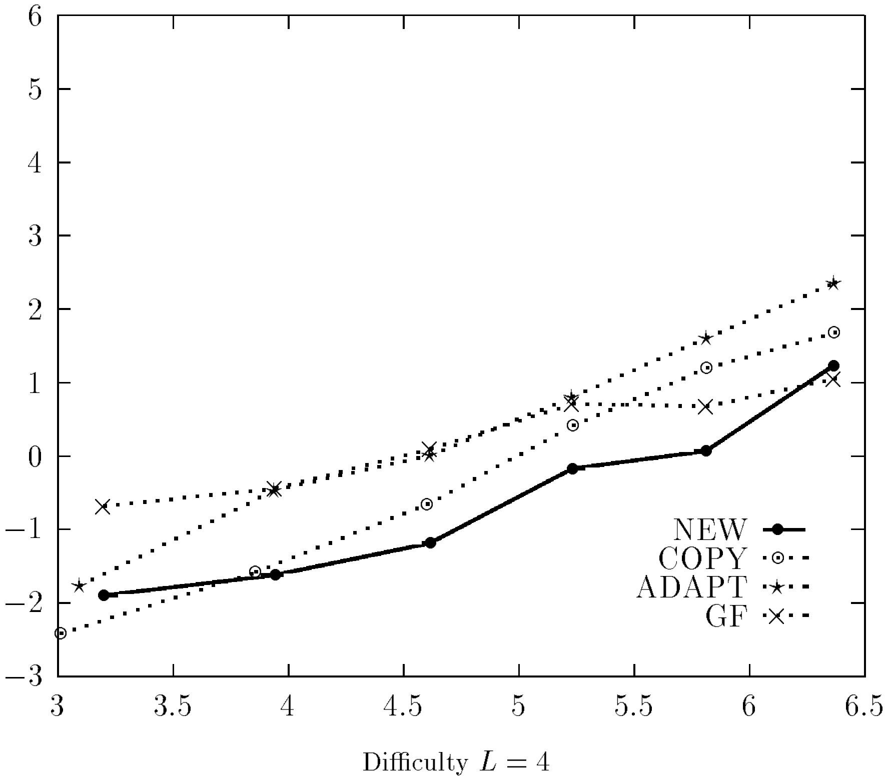
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Difficulty $L = 4$
NEW
COPY
ADAPT
GF

6. Rotated Genz Functions

Many cubature formulas depend on the underlying Cartesian coordinates. Examples include low discrepancy methods, ADAPT, NEW, and lattice rules like COPY. Hence one might suspect that formulas of the above type work particularly well for tensor product functions.

The Genz families 2, 4, 5, and 6 consist of tensor product functions. We use rotations to perturb this property. A natural fixed point is given by the vector w. We therefore consider functions

$$\widetilde{f}_i(x) = f_i(Q(x - w) + w)$$

for $i = 2, 4, 5, 6$ with orthogonal mappings Q on $\mathbb{R}^d$.

The exact computation of the integrals $\int_{[0,1]^d} \widetilde{f}_i(t)\, dt$ is difficult. Hence we only use successive twodimensional rotations, applied to disjoint pairs of variables. Then the integrals can be computed by means of twodimensional product formulas with sufficient accuracy.

We made a number of numerical tests for the methods ADAPT, COPY, and NEW with somewhat surprising results. All methods loose at most one correct digit in dimension $d = 10$. Up to this small difference the results do almost coincide with the results in Novak and Ritter (1996). Further details are presented in Schmitt (1996). It seems interesting to extend experiments to higher dimensional rotations.

7. Stopping Rules

On input ε an automatic integrator should stop if an error of at most ε is obtained for the first time. Clearly one cannot achieve this goal for every function. Instead one tries to work well in "most" cases. However, if additional properties of f are known, then one can construct stopping rules that work for every such function. See Förster (1993) for the case of univariate functions having some derivative of constant sign.

Let ε_r denote the relative accuracy that is demanded by the user. In order to handle cases of small or even zero integrals we also use a small absolute error bound $\varepsilon_a = 10^{-20}$, and we try to find a small q such that

$$|R(q, d)(f)| \le \varepsilon_a + \varepsilon_r \cdot |I(f)|.$$

We discuss a simple stopping rule for our algorithm, which is based on three consecutive values $A(q-2, d)(f)$, $A(q-1, d)(f)$, and $A(q, d)(f)$. We put

$$\Delta(q, d)(f) = |A(q, d)(f) - A(q-1, d)(f)|$$

and use the criterion

$$\Delta(q-1, d)(f) \le 10 \cdot \varepsilon_a + 800 \cdot \varepsilon_r \cdot A(q-1, d)(f)$$

and

$$\Delta(q, d)(f) \le \varepsilon_a + 35 \cdot \varepsilon_r \cdot A(q, d)(f).$$

We stop when these conditions hold for the first time.

We consider a stop at level q to be successful if

$$1/10 \cdot (\varepsilon_a + \varepsilon_r \cdot |I(f)|) \leq |R(q,d)(f)| \leq 10 \cdot (\varepsilon_a + \varepsilon_r \cdot |I(f)|).$$

We have checked the stopping rule for the Genz families 1–4 in dimensions 5, 8, and 10. For every family and dimension the rule worked successful in at least 3/4 of the examples. The constants in the stopping rules were found by numerical experiments.

To get better results we suggest to compute further approximations of $I(f)$ from the same set of knots that is used by $A(q,d)$. This can be done, for example, by replacing some formulas U_ℓ^i by U_ℓ^j for some $j < i$. The simplest case would be the following. Take a cubature formula $\widetilde{A}(q,d)$ that is based on the univariate formulas

$$U_\ell^1, \ldots, U_\ell^{q-d-1}, U_\ell^{q-d}, U_\ell^{q-d},$$

i.e., U_ℓ^{q-d+1} is replaced by U_ℓ^{q-d}. Now compare $A(q,d)$ with $\widetilde{A}(q,d)$. Observe that these formulas roughly use the same number of knots.

Stopping rules for the Smolyak method are also studied by Maerten (1996).

8. Applications in Physics, Statistics, and Finance

In this Section we report on integrands with Gaussian weight functions, because of their utility in a wide range of applications in physics, statistics, and finance. See Capstick and Keister (1996), Drmota and Tichy (1997), and Morokoff and Caflish (1995) for these and other examples. These integrals are of the form

$$\int_{\mathbb{R}^d} f(x) \exp(-\|x\|^2)\, dx. \tag{2}$$

Paskov and Traub (1995) introduce low discrepancy methods to evaluate collateralized mortgage obligations, see also Paskov (1996) and Caflish, Morokoff, and Owen (1997). One obtains integrals of the form (2). Although the dimension is very high, say $d = 360$, the integral can be computed with a relatively high accuracy by low discrepancy methods. Another complicated example is a Boltzmann collision integral of the form

$$\int_{\mathbb{R}^3}\int_0^{2\pi}\int_0^{\pi} f(\phi,\psi,x_1,x_2,x_3)\, \sin\phi\, \exp(-x_1^2 - x_2^2 - x_3^2)\, d\phi\, d\psi\, d(x_1,x_2,x_3), \tag{3}$$

see Morokoff and Caflish (1995).

It is not difficult to transform an integral of the form (2) or (3) to an integral over a bounded domain. For many methods such a transformation is actually necessary. However, the transformation can decrease the smoothness of the integrand extremely. The weight function in (3) is still a tensor product, but with different factors. Therefore fully symmetric quadrature formulas cannot be applied.

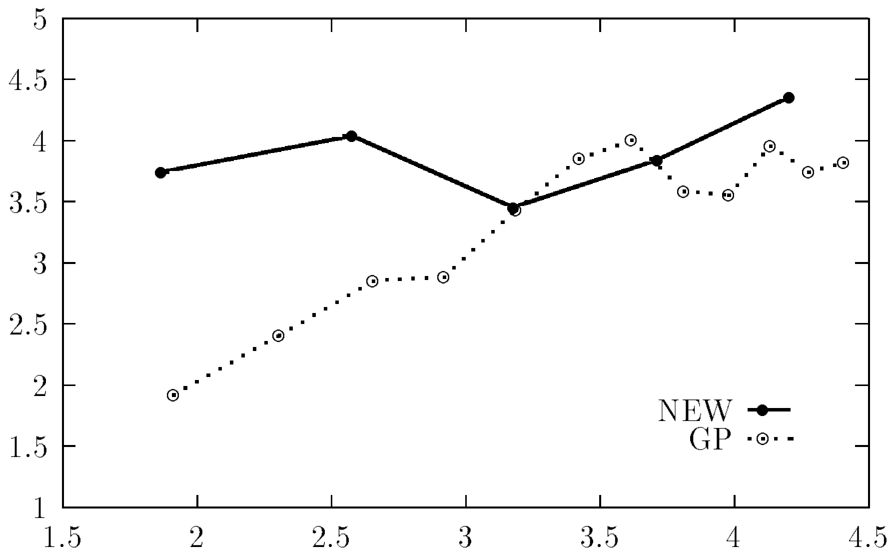
Our method can easily be applied to the integrals (2) or (3) directly. We can avoid a transformation and we can deal with different factors ϱ_i.

First we discuss the integral (2). In this case it is natural to use Gauss-Hermite formulas U^i. The resulting formula $A(q,d)$ is again denoted by NEW. We have considered the examples of Capstick and Keister (1996) which are of the form (2). These authors study fully symmetric formulas of McNamee and Stenger (1967) and Genz (1986). These formulas are denoted by MS and GP in the sequel. They are similar to $A(q,d)$ and also the results are similar – this is true in particular for the approach of Genz (1986). In the latter approach the efficiency is further improved by choosing knot values that cause certain sets of weights to vanish. To obtain such an "optimized" method one has to solve nonlinear equations. In contrast our method is quite explicit in the sense that we have simple algebraic expressions for the knots and the weights if the univariate formulas U_ℓ^i are given.

We present two examples, showing the number of correct digits versus $\log_{10} n$, as previously. The first one is given by

$$\int_{\mathbb{R}^d} \sqrt{1+\|x\|^2}\, \exp(-\|x\|^2)\, dx \tag{4}$$

with $d = 4$.

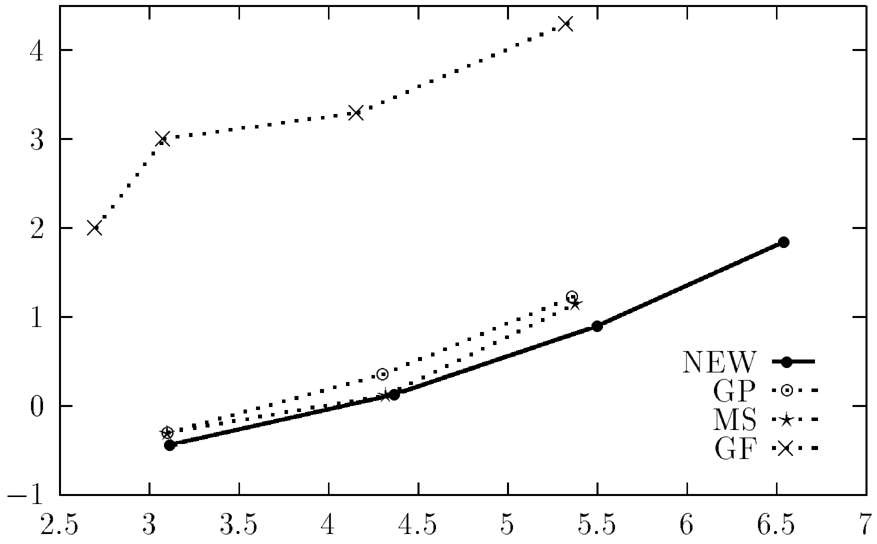


Function (4) with $d = 4$

Now we consider

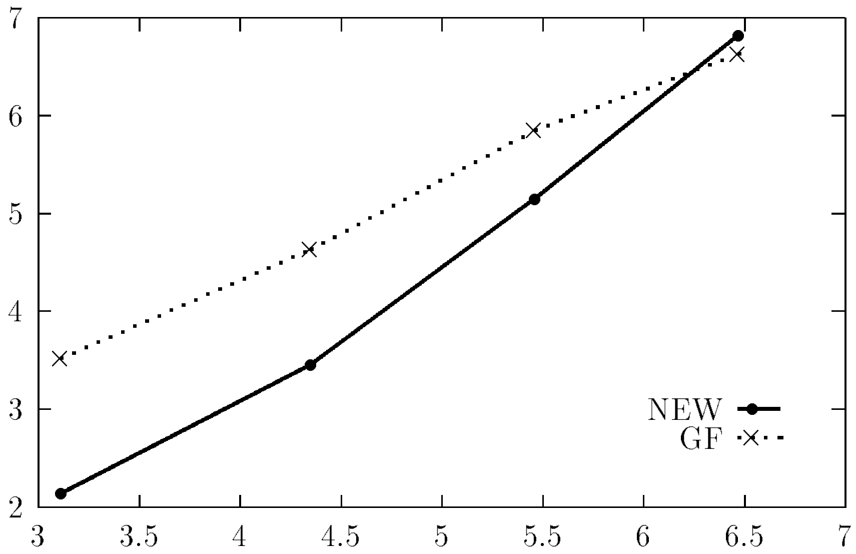
$$\int_{\mathbb{R}^d} \cos(\|x\|) \exp(-\|x\|^2)\, dx \tag{5}$$

with $d = 25$, see Capstick and Keister (1996) and Papageorgiou and Traub (1996). Since the dimension d is large we use the sequence $m_i = i$, i.e., we modify condition (A). The low discrepancy method GF performs extremely well.



Function (5) with $d = 25$

Another example with $d = 25$ is given by the family GAUSSIAN, see Section 4. We have chosen $\sum_{i=1}^{25} c_i = 10$. We did not make use of the structure of the integrand, but have used NEW with the Clenshaw Curtis formula and m_i as defined in (A). The following result is again based on 50 integrands, see Section 5.



Family GAUSSIAN with $d = 25$

For the integral (3) we suggest to use a method $A(q, d)$ (with $d = 5$) and the following ingredients:

- In the variable ϕ we have a weight function $\varrho_1 = \sin$ on the interval $[0, \pi]$. We use the sequence m_i as defined in (A), Chebyshev knots of the second kind, and weights as defined by (B). Hence (C) is fulfilled, too.
- Actually the integrand f is periodic in the variable ψ. Thus we take $m_i = 2^{i-1}$ and the midpoint rule. This choice of m_i leads to imbedded formulas. It is well known that the simple midpoint rule is optimal for many classes of periodic functions.
- For the remaining variables x_i we take Gauss-Hermite formulas.

We tried the resulting method with the function f from Morokoff and Caflish (1995). Our results are worse than the results for low discrepancy formulas that are described in that paper. The particular integral, however, is not smooth and therefore a fast convergence cannot really be expected.

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