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Computing Discrepancies Related to Spaces of
Smooth Periodic Functions

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Abstract

A notion of discrepancy is introduced, which represents the integration error on spaces of r -smooth periodic functions. It generalizes the diaphony and constitutes a periodic counterpart to the classical L_2 -discrepancy as well as r -smooth versions of it introduced recently by Paskov [Pas93]. Based on previous work [FH96], we develop an efficient algorithm for computing periodic discrepancies for quadrature formulas possessing certain tensor product structures, in particular, for Smolyak quadrature rules (also called sparse grid methods). Furthermore, fast algorithms of computing periodic discrepancies for lattice rules can easily be derived from well-known properties of lattices. On this basis we carry out numerical comparisons of discrepancies between Smolyak and lattice rules.

1 Introduction

Discrepancies are a quantitative measure of the precision of multivariate quadratures. Their computation, however, often is a very complex task. Therefore algorithms are of interest which reduce the cost of computing discrepancies either for general quadrature formulas or for special classes. The general case was treated in [War72], [Hei95], while in [FH96] the authors developed a technique of using tensor product structures of quadratures in order to speed up the computation of discrepancy. For the class of Smolyak quadratures, which was so far practically inaccessible to discrepancy computations, this supplied highly efficient algorithms. In [FH96] discrepancies and their behaviour under tensor products were studied in

a general setting involving arbitrary kernels on the unit cube. The resulting discrepancies turned out to be the worst case integration error over the unit ball of the corresponding reproducing kernel Hilbert spaces of functions. This general approach incorporates the classical L_2 -discrepancy and its r -smooth generalizations given by Paskov [Pas93]. It enabled us to compute these discrepancies for Smolyak quadratures and to compare them with known low discrepancy sequences as well as with standard Monte Carlo. For non-zero smoothness, the Smolyak rules performed very well. We refer to [FH96] for details.

The whole analysis of [FH96] was concerned with the non-periodic case (i. e. the corresponding reproducing kernel Hilbert spaces consist of non-periodic functions). On the other hand, an important class of multivariate quadratures — the class of lattice rules — was designed particularly for smooth periodic functions. Hence it would be desirable to have an analogue of the r -smooth discrepancy for the periodic case in order to compare lattice rules to other quadratures as e. g. Smolyak rules. The present paper is devoted to this task.

By using an appropriate kernel based on Bernoulli polynomials, we introduce the r -smooth periodic discrepancy $\widetilde{D}_r(Q)$ of a quadrature Q . It possesses natural interpretations — it is the worst case error of Q over the space of functions with square summable dominating mixed derivative of order r and the average error over a certain related Wiener measure. For smoothness $r = 1$, we recover the diaphony introduced in [Zin76], [ZS78]. Our approach provides an efficient algorithm for computing $\widetilde{D}_r(Q)$ for Smolyak quadratures Q . On the other hand, the well-known behaviour of lattice rules on Bernoulli polynomials provides also an efficient algorithm for computing \widetilde{D}_r for this type of quadrature.

As a consequence of this analysis, we are in a position to compare Smolyak and lattice rules numerically. We compare both of them with Monte Carlo integration (more precisely, with the easily explicitly computed expectation of \widetilde{D}_r of truly random points). Although Smolyak rules represent a very general approach which leads to optimal (up to logarithmic factors) rates on many classes of functions including those considered here — our experimental findings revealed a considerably better performance of lattice rules. Smolyak rules, in turn, are much better than Monte Carlo in the present situation.

Summarizing, we think that the periodic discrepancies are a further tool to work out the advantages or disadvantages of various classes of multivariate quadrature formulas.

The paper is organized as follows. In Section 2, we recall the Smolyak construction, Section 3 briefly explains the general approach to discrepancy developed in [FH96]. The periodic discrepancy is introduced in Section 4, while fast algorithms are given in Section 5. The final Section 6 contains the results of numerical experiments.

2 Smolyak quadratures

In 1963, Smolyak [Smo63] introduced a special tensor product technique which describes the construction of higher dimensional quadrature formulas and approximation operators on the basis of a sequence of the corresponding one-dimensional objects. If the one-dimensional methods involved possess some optimality features, this technique allows to achieve almost optimal error rates in higher dimensions, too. For an extensive list of references on theoretical investigations as well as on numerical experiments see [WW95] and [NR96].

Let $G = [0, 1]^d$. In the following we consider tensor products of quadrature formulas. Let $d = d_1 + d_2$, $d_1, d_2 \geq 1$, and $G = G_1 \times G_2$, with $G_1 = [0, 1]^{d_1}$, $G_2 = [0, 1]^{d_2}$. Let further Q', Q'' be quadrature formulas on G_1, G_2 , respectively,

$$Q' = ((x_{1j_1}, v_{1j_1}))_{j_1=1}^{M_1}, \quad Q'' = ((x_{2j_2}, v_{2j_2}))_{j_2=1}^{M_2},$$

and $Q = Q' \otimes Q'' = ((x_j, v_j) : j = (j_1, j_2), j_1 = 1, \dots, M_1, j_2 = 1, \dots, M_2)$ their standard tensor product

$$x_j = (x_{1j_1}, x_{2j_2}), \quad v_j = v_{1j_1} \cdot v_{2j_2}.$$

We want to approximate the d -dimensional integral

$$I f = \int_G f(x) dx,$$

where f is a continuous function on G . Given a sequence $(Q_n)_{n=0}^{\infty}$ of one-dimensional quadrature rules on $[0, 1]$ for continuous functions $f \in C([0, 1])$,

$$Q_n f = \sum_{j=1}^{P_n} w_j^n \cdot f(x_j^n),$$

with $w_j^n \in \mathbb{R}$, $x_j^n \in [0, 1]$, we construct the standard tensor product quadrature for the approximate computation of $I f$ as

$$U_n^{(d)} f = (Q_n \otimes U_n^{(d-1)}) f = \sum_{j=0}^n (Q_j - Q_{j-1}) \otimes U_n^{(d-1)} f,$$

where $U_n^{(1)} = Q_n$, $Q_{-1} \equiv 0$. Smolyak's approach modifies this definition, setting $Q_n^{(1)} = Q_n$ and defining recursively (see [Smo63])

$$Q_n^{(d)} f = \sum_{j=0}^n (Q_j - Q_{j-1}) \otimes Q_{n-j}^{(d-1)} f, \quad (1)$$

where again $Q_{-1} \equiv 0$. The point set $\Gamma_n^{(d)}$ exploited by the quadrature $Q_n^{(d)}$ is a so-called sparse grid. As was derived in [FH96], its cardinality can be calculated recursively by the formula

$$|\Gamma_n^{(d)}| = \sum_{j=0}^n |\Gamma_j^{(1)} \setminus \Gamma_{j-1}^{(1)}| \cdot |\Gamma_{n-j}^{(d-1)}|, \quad (2)$$

where $\Gamma_{-1}^1 = \emptyset$, provided that the one-dimensional grids $\Gamma_j^{(1)}$ are nested, that means $\Gamma_0^{(1)} \subset \Gamma_1^{(1)} \subset \dots \subset \Gamma_n^{(1)}$. This condition will be satisfied in all concrete realizations of Smolyak rules we consider in this paper. Note that in contrast to the total number of points in a regular tensor product grid $N = O(M_n^d)$, under some natural assumptions on the sequence (M_n) , the number of points in the sparse grid $\Gamma_n^{(d)}$ is reduced to $|\Gamma_n^{(d)}| = O(M_n(\log M_n)^{d-1})$.

3 A general approach to discrepancy

Here we recall the definition of discrepancies related to arbitrary reproducing kernel Hilbert spaces as given in [FH96]. In fact, we choose a formally slightly more general presentation which, however, is equivalent to that in [FH96]. This equivalence follows from Mercer's Theorem, see the argument in [FH96, Section 3].

Let $G = [0, 1]^d$, let H be an arbitrary real Hilbert space, and let $C(G, H)$ denote the space of continuous functions from G into H (where H is endowed with the norm topology). Fix a function $B(x)$ ($x \in G$) with $B \in C(G, H)$. For this B we define a discrepancy D_B as follows. Let $Q = ((x_1, v_1), \dots, (x_M, v_M))$ be a quadrature formula on G , i. e. $x_j \in G$, $v_j \in \mathbb{R}$ ($j = 1, \dots, M$). Put

$$IB = \int_G B(x) dx$$

(the Bochner integral) and

$$QB = \sum_{j=1}^M v_j B(x_j).$$

Then the discrepancy $D_B(Q)$ is defined as

$$D_B(Q) = \|IB - QB\|_H. \quad (3)$$

Hence we get

$$\begin{aligned} D_B(Q)^2 &= (IB - QB, IB - QB) \\ &= C_B - 2F_B(Q) + S_B(Q, Q), \end{aligned} \quad (4)$$

where (\cdot, \cdot) is the scalar product in H and we used the notation

$$C_B = (IB, IB) \tag{5}$$

$$F_B(Q) = (IB, QB) \tag{6}$$

$$S_B(Q, R) = (QB, RB). \tag{7}$$

Here R can be any quadrature on G , $R = ((y_1, w_1), \dots, (y_N, w_N))$. It follows readily from (3) that $D_B(Q)$ is the worst-case integration error of the quadrature Q over the function class

$$W_B = \{g \in C(G) : \exists h \in H, \|h\|_H \leq 1 : \forall x \in G : g(x) = (B(x), h)\}. \tag{8}$$

Here $C(G)$ denotes the space of continuous real functions on G . Setting $K(x, y) = (B(x), B(y))$, $x, y \in G$, we get a continuous, symmetric, non-negative definite function on G^2 , and the class W_B is the unit ball of the reproducing kernel Hilbert space generated by K . Finally, if μ is the mean-zero Gaussian measure on $C(G)$ with covariance kernel K , $D_B(Q)$ is the average case quadrature error of Q with respect to μ (see [SY70]).

From now on we set $H = L_2(G)$, the space of square-integrable functions with respect to the Lebesgue measure. Hence we consider functions $B(x, t)$ on G^2 which are such that $B(x, \cdot) \in L_2(G)$ and $B(x) = B(x, \cdot)$ is continuous from G to $L_2(G)$. In [FH96], the special case $B(x, t) = \frac{1}{(r!)x}(t-x)_+^r$ was studied, where r is a non-negative integer and $a_+ = a$ if $a > 0$ and $a_+ = 0$ otherwise. For $r = 0$ this gives the classical L_2 -discrepancy, while for $r > 0$ one gets the r -smooth versions introduced by Paskov [Pas93]. The resulting classes W_B are unit balls of Sobolev spaces of functions with L_2 -bounded dominating mixed derivative, which satisfy certain (non-periodic) boundary conditions (see [FH96], [Pas93]). In this paper we shall consider the periodic case, which will be introduced in the next section.

4 Discrepancies related to Sobolev spaces of periodic functions

Let $r > 0$ be a natural number. Define for $x \in \mathbb{R}$

$$p_r(x) = 1 - (-1)^{\lfloor \frac{x}{2} \rfloor} \frac{(2\pi)^r}{r!} b_r(x)$$

where $b_r(x)$ denotes the r -th Bernoulli polynomial, and $[a]$ is the largest integer not exceeding a . It is well-known (see e. g. [GR65, 9.622, 9.623.3]) that for $x \in \mathbb{R}$,

$$p_r(\{x\}) = 1 + 2 \sum_{n=1}^{\infty} n^{-r} \cos 2\pi n x$$

if r is even, and

$$p_r(\{x\}) = 1 + 2 \sum_{n=1}^{\infty} n^{-r} \sin 2\pi n x$$

if r is odd. Here $\{a\} = a - [a]$ is the fractional part of a number $a \in \mathbb{R}$. For $r \geq 2$ the series converge absolutely and uniformly, for $r = 1$ it converges in $L_2([0, 1])$. Now define for $x = (\xi_1, \dots, \xi_d) \in \mathbb{R}^d$

$$P_r(x) = \prod_{l=1}^d p_r(\xi_l)$$

and for $x, t \in G$, $x = (\xi_1, \dots, \xi_d)$, $t = (\tau_1, \dots, \tau_d)$,

$$B_r^{(d)}(x, t) = P_r(\{x - t\}),$$

where $\{x - t\} = (\{\xi_1 - \tau_1\}, \dots, \{\xi_d - \tau_d\})$. Although we deal with real functions only, it is convenient for us to use the following representation

$$p_r(\{x\}) = \sum_{n \in \mathbb{Z}} \sigma_r(n) \bar{n}^{-r} e^{2\pi i n x}, \quad (9)$$

where $\bar{n} = |n|$ if $n \neq 0$, $\bar{n} = 1$ if $n = 0$, and

$$\sigma_r(n) = \begin{cases} -\text{sign}(n) i & \text{if } n \neq 0 \text{ and } r \text{ is odd,} \\ 1 & \text{otherwise.} \end{cases}$$

For $n = (n_1, \dots, n_d)$ we set

$$\bar{n} = \prod_{l=1}^d \bar{n}_l, \quad \sigma_r(n) = \prod_{l=1}^d \sigma_r(n_l).$$

Hence we get for $x, t \in G$

$$B_r^{(d)}(x, t) = \sum_{n \in \mathbb{Z}^d} \sigma_r(n) \bar{n}^{-r} e^{2\pi i (n, x - t)}. \quad (10)$$

It is easily derived from these representations and from (8) that $W_{B_r^{(d)}}$ is the unit ball of the Sobolev space of real functions

$$\mathcal{H}^r(G) = \{g \in L_2(G) : \|g\|_r^2 = \sum_{n \in \mathbb{Z}^d} \bar{n}^{2r} |\hat{g}(n)|^2 < \infty\}$$

where

$$\hat{g}(n) = \int_G g(t) e^{-2\pi i n t} dt$$

is the n -th Fourier coefficient (see e. g. [Fra95], where this space is considered). $\mathcal{H}^r(G)$ consists of all periodic functions $g \in L_2(G)$ whose generalized derivatives

$$\frac{\partial^{\alpha_1 + \dots + \alpha_d} g(\xi_1, \dots, \xi_d)}{\partial \xi_1^{\alpha_1} \dots \partial \xi_d^{\alpha_d}}$$

belong to $L_2(G)$ whenever $0 \leq \alpha_l \leq r$ ($l = 1, \dots, d$). Let us now consider the discrepancy defined by (3) and (4) on the basis of the function $B_r^{(d)}(x, t)$. Let $Q = ((x_j, v_j))_{j=1}^M$, $R = ((y_j, w_j))_{j=1}^N$ and denote

$$\begin{aligned} \widetilde{D}_r(Q) &= D_{B_r^{(d)}}(Q); \\ \widetilde{S}_r(Q, R) &= S_{B_r^{(d)}}(Q, R), \quad \widetilde{F}_r(Q) = F_{B_r^{(d)}}(Q), \quad \widetilde{C}_r = C_{B_r^{(d)}}. \end{aligned}$$

In these notations, for the sake of simplicity we drop the dimension parameter, which is indicated by the arguments Q, R . By the discussion above, $\widetilde{D}_r(Q)$ is the worst case error of a quadrature Q over the unit ball of the space $\mathcal{H}^r(G)$. We consider the representation (4) and compute each of the terms. Using (9) and (10) we easily obtain

$$\widetilde{C}_r = 1, \quad \widetilde{F}_r(Q) = \sum_{j=1}^M v_j, \tag{11}$$

and

$$\begin{aligned} \widetilde{S}_r(Q, R) &= \sum_{j=1}^M \sum_{k=1}^N v_j w_k \sum_{m \in \mathbb{Z}^d} \bar{m}^{-2r} e^{2\pi i(m, x_j - y_k)} \\ &= \sum_{j=1}^M \sum_{k=1}^N v_j w_k P_{2r}(\{x_j - y_k\}) \end{aligned} \tag{12}$$

It follows that $\widetilde{D}_r(Q)$ can be computed in $O(M^2)$ operations. Below we analyze situations, in which this can be done in a faster way. Note that for $r = 1$ and

uniform weights $v_j = 1/M$ ($j = 1, \dots, M$), $\widetilde{D}_1(Q)$ is the diaphony of the point set $(x_j, j = 1, \dots, M)$ introduced and studied in [Zin76] and [ZS78]. To see this, observe that (4), (11) and (12) give for the case of weights satisfying $\sum_{j=1}^M v_j = 1$,

$$\widetilde{D}_r(Q)^2 = \sum_{j,k=1}^M v_j v_k \left(\prod_{l=1}^d p_{2r}(\{x_{jl} - x_{kl}\}) - 1 \right).$$

It remains to compare $p_{2r}(\{x\})$ with the function $g(x)$ of [ZS78].

5 Fast computation of $\widetilde{D}_r(Q)$

The recursive approach of [Hei95] could be applied to develop an algorithm for the computation of $\widetilde{D}_r(Q)$. Formally, this would lead to an $O(M(\log M)^d)$ algorithm as in [Hei95, Section 4], but with a heavy dependence of the constants on r and d . So only small r and d can be handled. In this section we concentrate on special types of quadratures — good lattice points and Smolyak rules.

Let L be a d -dimensional integration lattice (see [Nie92, Section 5.3]) and let Q_L be the associated quadrature rule on G with node set $L \cap G'$, $G' = [0, 1]^d$, and uniform weights. The computation of $\widetilde{D}_r(Q_L)$ is easily accomplished following the lines of the analysis for the Korobov classes \mathcal{E}_r^d (see [Kor63], [Nie92, Th. 5.23]). According to Lemma 5.21 of [Nie92] we have

$$Q_L e^{2\pi i(n, \cdot)} = \begin{cases} 1 & \text{if } n \in L^\perp \\ 0 & \text{if } n \notin L^\perp, \end{cases}$$

where $L^\perp = \{n \in \mathbb{Z}^d : (n, x) \in \mathbb{Z} \text{ for all } x \in L\}$ is the dual lattice. Using this, the definition (3) and relation (10), we get

$$\begin{aligned} \widetilde{D}_r(Q_L) &= \|IB_r^{(d)} - Q_L B_r^{(d)}\|_{L_2(G)} \\ &= \left\| \sum_{n \in \mathbb{Z}^d} \sigma_r(n) \bar{n}^{-r} \left((I - Q_L) e^{2\pi i(n, \cdot)} \right) e^{-2\pi i(n, t)} \right\|_{L_2(G)} \\ &= \left(\sum'_{n \in L^\perp} \bar{n}^{-2r} \right)^{1/2} = \left| (I - Q_L) B_{2r}^{(d)}(\cdot, 0) \right|^{1/2} \end{aligned} \quad (13)$$

As usual, \sum' means that the summand for $n = (0, \dots, 0)$ is left out. Hence in order to compute $\widetilde{D}_r(Q_L)$ we have to determine the integration error of Q_L on the single function

$$B_{2r}^{(d)}(x, 0) = P_{2r}(x) = \prod_{l=1}^d p_{2r}(\xi_l), \quad x = (\xi_1, \dots, \xi_d) \in G'.$$

This is just the number theorists criterion considered in various papers dedicated to the search of optimal parameters for good lattice points, e. g. [Hab83], [SW90]. The evaluation of the integration error on $P_{2r}(x)$ is an $O(M)$ procedure. Note that (13) and Theorem 5.23 of [Nie92] imply that for lattice rules Q_L

$$\sup_{f \in B_{\mathcal{H}^r}} |(I - Q_L)f| = \sup_{g \in B_{\mathcal{E}_r^d}} |(I - Q_L)g|^{1/2}$$

where B_X denotes the unit ball of the space X , and the Korobov space \mathcal{E}_r^d consists of all functions $g \in L_2(G)$ with

$$\|g\|_{\mathcal{E}_r^d} = \sup_{n \in \mathbb{Z}^d} \bar{n}^{-r} |\hat{g}(n)| < \infty.$$

Next we consider Smolyak quadratures. In [FH96], we developed a recursive algorithm which allows to reduce the computation of D_B to the one-dimensional case provided $B(x, t)$ has product structure. This result applies to the present situation. The algorithm is the following.

As introduced in Section 2, the Smolyak quadrature rule on $[0, 1]^d$, $d \geq 2$, satisfies the recursion

$$Q_n^{(d)} = \sum_{i=0}^n R_i \otimes Q_{n-i}^{(d-1)},$$

where $R_i = Q_i - Q_{i-1}$, $Q_{-1} \equiv 0$ and $Q_n^{(1)} = Q_n$. We fix a maximal level n_{max} and apply a recursion over d to calculate all quantities $\tilde{F}_r(Q_n^{(d)})$ and $\tilde{S}_r(Q_m^{(d)}, Q_n^{(d)})$ for $m, n = 0, 1, \dots, n_{max}$.

The recursion starts from the univariate case by computing the terms $\tilde{F}_r(Q_n)$, $\tilde{S}_r(Q_m, Q_n)$. From these terms we get using the behavior of \tilde{F}_r and \tilde{S}_r under sums and tensor products as established in [FH96]

$$\begin{aligned} \tilde{F}_r(R_n) &= \tilde{F}_r(Q_n) - \tilde{F}_r(Q_{n-1}) \\ \tilde{S}_r(R_m, R_n) &= \tilde{S}_r(Q_m, Q_n) - \tilde{S}_r(Q_{m-1}, Q_n) \\ &\quad - \tilde{S}_r(Q_m, Q_{n-1}) + \tilde{S}_r(Q_{m-1}, Q_{n-1}) \\ \tilde{F}_r(Q_n^{(d)}) &= \sum_{i=0}^n \tilde{F}_r(R_i) \cdot \tilde{F}_r(Q_{n-i}^{(d-1)}) \\ \tilde{S}_r(Q_m^{(d)}, Q_n^{(d)}) &= \sum_{i=0}^m \sum_{j=0}^n \tilde{S}_r(R_i, R_j) \cdot \tilde{S}_r(Q_{m-i}^{(d-1)}, Q_{n-j}^{(d-1)}) \end{aligned}$$

Finally, the discrepancy $\tilde{D}_r(Q_n^{(d)})$ is given by (4), where by (11) $\tilde{C}_r = 1$ independently of the dimension.

To handle the one-dimensional quantities, let $Q = ((x_j, v_j))_{j=1}^M$ and $R = ((y_k, w_k))_{k=1}^N$ be quadratures on $[0, 1]$. It is sufficient to transform $\tilde{S}_r(Q, R)$ into an efficiently computable form, since $\tilde{F}_r(Q)$ can be calculated in $O(M)$ operations simply by (11). We assume that the node sets are ordered in such a way that $x_1 \leq x_2 \leq \dots \leq x_M$ and $y_1 \leq y_2 \leq \dots \leq y_N$. Let us mention that the node sets of many quadrature rules are ordered by their definition. Then we determine for each $j = 1, \dots, M$ an index $\nu(j)$ such that $x_j \geq y_k$ for each $k \leq \nu(j)$ and $x_j < y_k$ for $k > \nu(j)$. Using this we can rewrite the direct formula (12) as follows

$$\begin{aligned}\tilde{S}_r(Q, R) &= \sum_{j=1}^M \sum_{k=1}^N v_j w_k p_{2r}(\{x_j - y_k\}) \\ &= \sum_{j=1}^M v_j \sum_{k=1}^N w_k - (-1)^r \frac{(2\pi)^{2r}}{(2r)!} \varphi^{(r)}\end{aligned}$$

where

$$\begin{aligned}\varphi^{(r)} &= \sum_{j=1}^M v_j \left[\sum_{k=1}^{\nu(j)} w_k b_{2r}(x_j - y_k) + \sum_{k=\nu(j)+1}^N w_k b_{2r}(1 + x_j - y_k) \right] \\ &= \sum_{l=0}^{2r} \alpha_{l,2r} \sum_{q=0}^l \binom{l}{q} \sum_{j=1}^M v_j x_j^{l-q} * \\ &\quad * \left[\sum_{k=1}^{\nu(j)} w_k (-y_k)^q + \sum_{k=\nu(j)+1}^N w_k (1 - y_k)^q \right]\end{aligned}\tag{14}$$

Here $\alpha_{l,2r} \in \mathbb{R}$ are the coefficients of the Bernoulli polynomial b_{2r}

$$b_{2r}(x) = \alpha_{0,2r} + \alpha_{1,2r}x + \dots + \alpha_{2r,2r}x^{2r}.$$

Both sums in (14) can be calculated in $O(M + N)$, if the inner sums are added up successively. We fix $r \geq 0$. Assume that there are reals $p > 1$, $c_1, c_2 > 0$ such that the number of nodes P_n in the one-dimensional quadratures Q_n satisfies

$$c_1 p^n \leq P_n \leq c_2 p^n.$$

This is a natural assumption for Smolyak quadratures. Fix n_{max} and denote $P = P_{n_{max}}$. Obviously, $n_{max} = O(\log P)$. As was pointed out in [FH96], the complexity of the whole recursion process is then $O(P \log P + d(\log P)^4)$.

6 Numerical results

We will compare the L_2 -discrepancies \widetilde{D}_r of two different Smolyak quadrature rules with rank-1 lattices, rank-2 lattices and Monte Carlo integration.

The Smolyak rules are fully determined by the recursion (1) and the sequence (Q_n) ($n = 0, \dots, n_{max}$) of one-dimensional quadratures. We will test two sequences used already in [FH96]. In both quadratures Q_0 is chosen as the midpoint rule

$$Q_0 f = f(0.5),$$

because otherwise the number of grid points would increase exponentially in d . As sequence (Q_n) ($n \geq 1$) of one-dimensional rules the Smolyak rule TR uses the sequence of composite trapezoidal rules on 2^n subintervals, whereas CC takes the sequence of Clenshaw-Curtis rules using 2^n subintervals (see [Bra77]). Note that by (2) the exact number of sample points employed by $Q_n^{(d)}$ coincides in both cases.

To compare Monte Carlo integration, we do not use any concrete random number generator, but compute the square mean of the discrepancy \widetilde{D}_r

$$\begin{aligned} \mathbb{E} \widetilde{D}_r(Q)^2 &= \mathbb{E} \int_G \left(IB_r^{(d)}(\cdot, t) - \frac{1}{M} \sum_{i=1}^M B_r^{(d)}(\zeta_i, t) \right)^2 dt \\ &= \frac{1}{M} \int_G \mathbb{E} \left(IB_r^{(d)}(\cdot, t) - B_r^{(d)}(\zeta_1, t) \right)^2 dt \\ &= \frac{1}{M} \int_G \left(\int_G B_r^{(d)}(x, t)^2 dx - \left(\int_G B_r^{(d)}(x, t) dx \right)^2 \right) dt \\ &= \frac{1}{M} \left(B_{2r}^{(d)}(0, 0) - 1 \right). \end{aligned}$$

Finally, we include lattice rules into our comparisons. This family of quadrature formulas was developed by Korobov [Kor63] and Hlawka [Hla62], and is designed especially for the integration of periodic functions of several variables. We will consider lattice rules of rank 1 with parameters as indicated in [Hab83], and lattice rules of rank 2 with parameters from [SW90].

All computations were carried out on a workstation of the series HP-9000 in the language C⁺⁺. Due to cancellation in (4) it was necessary to use quadruple precision.

Unfortunately, the parameters for the good-lattice points were given only for certain numbers of points in [Hab83] and [SW90]. Neither can the number of sample points in the Smolyak quadratures be chosen voluntarily but depends on the dimension and the maximal level n_{max} . We tried to select such parameter combinations that the quadrature rules compared in one table work with as similar numbers of function values as possible. To be just against the Monte Carlo quadrature we computed

r	CC	TR	Rank 1	Rank 2	MC
	13953	13953	12288	10404	13953
1	3.39e-01	2.08e-01	1.14e-02	9.64e-03	7.47e-02
2	4.91e-03	1.09e-03	2.70e-05	1.03e-05	4.69e-02
3	1.44e-04	8.18e-06	8.86e-08	1.48e-08	4.40e-02
4	5.98e-06	6.34e-08	3.06e-10	2.28e-11	4.34e-02

r	CC	TR	Rank 1	Rank 2	MC
	18945	18945	16384	10332	18945
1	2.51	1.88	3.97e-02	4.63e-02	1.34e-01
2	1.63e-01	3.21e-02	2.08e-04	2.08e-04	7.24e-02
3	3.48e-02	9.31e-04	1.59e-06	1.33e-06	6.65e-02
4	1.34e-02	2.87e-05	1.33e-08	9.40e-09	6.53e-02

Table 1: Discrepancies with $M \approx 10^4$ points in $d = 3$ (top) and $d = 4$ (bottom)

the square mean of its discrepancy always with the highest number of points in the respective table. However, its performance turned out to be poor in comparison with the other methods.

Tables 1-3 report some numerical experiments for $M \approx 10^4$ (Table 1) and $M \approx 10^5$ (Tables 2, 3). The results almost speak for themselves. In contrast to [FH96], the Smolyak quadratures do not perform very well, particularly with moderate numbers of grid points in higher dimensions. Among them only the Smolyak quadrature based on the trapezoidal rule can achieve satisfactory results. This is due to the fact, that the trapezoidal rule is optimal on the class of smooth periodic functions on $[0, 1]$ (see [TWW88]).

Since good-lattice points were developed especially for periodic functions of several variables, it was to be expected that their discrepancy would be smaller than the discrepancy of the tensor product methods. However, we were surprised by the extend of superiority of the number-theoretic methods. As is only natural, the

r	CC	TR	Rank 1	Rank 2	MC
	127105	127105	131072	100044	131072
1	37.42	43.05	1.18e-01	1.03e-01	2.18e-01
2	3.38	1.47	1.67e-03	8.04e-04	8.75e-02
3	1.37	1.33e-01	4.01e-05	1.15e-05	7.71e-02
4	8.89e-01	1.51e-02	1.05e-06	1.85e-07	7.51e-02

Table 2: Discrepancies with $M \approx 10^5$ points in $d = 6$

r	CC	TR	Rank 1	Rank 2	MC
	163841	163841	131072	100044	131072
1	6.16e-02	3.51e-02	1.53e-03	1.54e-03	2.18e-02
2	1.12e-04	2.31e-05	6.08e-07	3.25e-07	1.37e-02
3	3.84e-07	2.16e-08	3.29e-10	9.24e-11	1.28e-02
4	1.78e-09	2.09e-11	1.84e-13	2.83e-14	1.26e-02

r	CC	TR	Rank 1	Rank 2	MC
	113409	113409	131072	100044	131072
1	1.01	6.46e-01	8.04e-03	7.86e-03	5.08e-02
2	1.82e-02	2.89e-03	1.15e-05	6.14e-06	2.75e-02
3	9.31e-04	2.12e-05	2.44e-08	6.90e-09	2.53e-02
4	8.54e-05	1.64e-07	5.48e-11	8.54e-12	2.48e-02

Table 3: Discrepancies with $M \approx 10^5$ points in $d = 3$ (top) and $d = 4$ (bottom)

more general rank-2 methods showed even a slightly better performance than the rank-1 rules.

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