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ON COMPUTING THE LATTICE RULE CRITERION R

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ABSTRACT. Lattice rules are integration rules for approximating integrals of periodic functions over the s-dimensional unit cube. One criterion for measuring the 'goodness' of lattice rules is the quantity R. This quantity is defined as a sum which contains about N^{s-1} terms, where N is the number of quadrature points. Although various bounds involving R are known, a procedure for calculating R itself does not appear to have been given previously. Here we show how an asymptotic series can be used to obtain an accurate approximation to R. Whereas an efficient direct calculation of R requires $O(Nn_1)$ operations, where n_1 is the largest 'invariant' of the rule, the use of this asymptotic expansion allows the operation count to be reduced to $O(N)$. A complete error analysis for the asymptotic expansion is given. The results of some calculations of R are also given.

1. INTRODUCTION

Lattice rules were developed in [15, 16, and 17] for the numerical evaluation of integrals of the form

$$If = \int_{U^s} f(\mathbf{x})\,d\mathbf{x},$$

where

$$U^s = \{\mathbf{x} \in \mathbb{R}^s : 0 \le x_k < 1,\ \ 1 \le k \le s\}$$

is the half-open unit cube in s dimensions, and f is assumed to be 1-periodic in each of its s variables. Lattice rules are equal-weight rules of the form

$$(1.1) \qquad Qf = \frac{1}{N}\sum_{j=0}^{N-1} f(\mathbf{x}_j),$$

in which the abscissa set $\{\mathbf{x}_0, \dots, \mathbf{x}_{N-1}\}$ consists of all the points in U^s that also belong to a given 'integration lattice'. A lattice is a discrete set of points in $\mathbb{R}^s$ such that the sum and difference of every point in the set also belongs to the set; the lattice is an integration lattice if it contains the integer lattice $\mathbb{Z}^s$ as a sublattice. A lattice rule with N distinct abscissae is said to be of order N.

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The representation of lattice rules has been discussed extensively in [18]. There, we find the result that every lattice rule may be written as an expression of the form

$$(1.2) \qquad Qf = \frac{1}{N}\sum_{j_m=0}^{n_m-1}\cdots\sum_{j_1=0}^{n_1-1} f\left(\frac{j_1}{n_1}\mathbf{z}_1 + \cdots + \frac{j_m}{n_m}\mathbf{z}_m\right),$$

where n_{k+1} divides n_k for $k = 1, \dots, m-1$, $n_m \geq 2$, and $N = n_1 n_2 \cdots n_m$ is the order of the rule. The number m, which satisfies $1 \leq m \leq s$, is known as the 'rank' of the rule and $n_1, \dots, n_m$ are the 'invariants'. (The abscissae as they appear in (1.2) may not lie in U^s, but equivalent abscissae that do lie in U^s may be obtained by subtraction of appropriate integer vectors: for the assumed periodicity of f ensures that this subtraction leaves the lattice rule unchanged.)

Lattice rules generalize the well-studied method of good lattice points due to Korobov [10] and Hlawka [6], in which the rule is of the rank-1 form

$$(1.3) \qquad Qf = \frac{1}{N}\sum_{j=0}^{N-1} f\left(\frac{j}{N}\mathbf{z}\right).$$

Here, $\mathbf{z}$ is a integer vector of length s having no nontrivial factor common with N.

The error in the lattice rule Q is easily stated.

Theorem 1 [17]. *Suppose Q is the lattice rule* (1.1) *and f has the absolutely convergent Fourier series representation*

$$f(\mathbf{x}) = \sum_{\mathbf{h}\in\mathbb{Z}^s} a(\mathbf{h})e^{i2\pi\mathbf{h}\cdot\mathbf{x}}.$$

Then

$$(1.4) \qquad Qf - If = \sum_{\mathbf{h}\in L^\perp}{}' \, a(\mathbf{h}).$$

In the theorem, $\mathbf{h}\cdot\mathbf{x}$ is the usual inner product in s dimensions, the prime on the sum indicates that the $\mathbf{h} = \mathbf{0}$ term is omitted, and $L^\perp$ is the 'dual lattice' defined by

$$L^\perp := \{\mathbf{h} \in \mathbb{Z}^s : \mathbf{h}\cdot\mathbf{x}_k \in \mathbb{Z},\ 0 \leq k \leq N-1\};$$

it is the dual of the lattice $L(Q)$ which corresponds to Q.

There are several criteria available for measuring the 'goodness' of a lattice rule, all coming from the number-theoretic literature associated with the method of good lattice points. One such criterion is given by P_α, where for fixed $\alpha > 1$,

$$P_\alpha = P_\alpha(Q) := \sum_{\mathbf{h}\in L^\perp}{}' \frac{1}{(\bar{h}_1\bar{h}_2\cdots\bar{h}_s)^\alpha},$$

with

$$\bar{h} = \max(1, |h|).$$

This criterion has been used extensively (for instance, see [1, 2, 3, 5, 8, 9, 12, 14, 17, and 19]). It is evident from (1.4) that P_α is just $Qf_\alpha - If_\alpha = Qf_\alpha - 1$, where

$$f_\alpha(\mathbf{x}) = \sum_{\mathbf{h}\in\mathbb{Z}^s} \frac{e^{i2\pi\mathbf{h}\cdot\mathbf{x}}}{(\bar{h}_1\bar{h}_2\cdots\bar{h}_s)^\alpha}.$$

Another criterion that has been used is the quantity R (see [13 and 14]), which for a lattice rule of order N is given by

$$R = R(Q) := \sum_{\mathbf{h}\in L^{\perp}\cap\mathbf{E}(N)}{}' \frac{1}{\bar{h}_1\bar{h}_2\cdots\bar{h}_s}, \tag{1.5}$$

where

$$\mathbf{E}(N) = \{\mathbf{h}\in\mathbb{Z}^s:\ -N/2 < h_k \le N/2,\ 1\le k\le s\}.$$

However, a procedure for calculating this quantity does not appear to have been given previously. Now, because L has N points per unit volume, the average density of points in $L^{\perp}$ is $1/N$ (see [17]) and $\mathbf{E}(N)$ has volume N^s. Thus, the sum in (1.5) contains about N^{s-1} terms. It follows that it would not in general be practical to use (1.5) directly to calculate R. In §2 and §3 we give an alternative method that enables R to be calculated efficiently for any lattice rule.

Our approach makes use of the fact that, from (1.4),

$$R(Q) = Qf_N - If_N = Qf_N - 1,$$

where

$$f_N(\mathbf{x}) = \sum_{\mathbf{h}\in\mathbf{E}(N)} \frac{e^{i2\pi\mathbf{h}\cdot\mathbf{x}}}{\bar{h}_1\bar{h}_2\cdots\bar{h}_s} = \prod_{k=1}^{s} F_N(x_k),$$

with

$$F_N(x) = \sum_{-N/2<h\le N/2} \frac{e^{i2\pi hx}}{\bar{h}} = 1 + \sum_{h\in E^*(N)} \frac{e^{i2\pi hx}}{|h|},$$

and $E^*(N) := \{h\in\mathbb{Z} : -N/2 < h \le N/2,\ h\ne 0\}$. (This approach was followed previously by Korobov [11, Chapter 3] in the method of good lattice points, as a way of obtaining bounds on $R(Q)$.)

Since F_N has N terms and the lattice rule also has N terms, we see that a direct calculation of R by the above formulae, in which for each point $\mathbf{x} = (x_1, \ldots, x_s)$ of the lattice rule one calculates $F_N(x_1), \ldots, F_N(x_s)$ and then their product, would (for fixed s) require $O(N^2)$ operations. Actually, this number can be reduced by calculating in advance all of the values of F_N which are required. For the rule with invariants $n_1, \ldots, n_m$ (see (1.2)), it is easy to see that it is sufficient to calculate only the values $F_N(j/n_1)$, $j = 0, \ldots, n_1-1$, where n_1 is the largest invariant. Organized this way, the calculation requires only $O(Nn_1)$ operations. The most favorable case is the product-rectangle rule in which $m = s$ and $n_1 = \cdots = n_s = N^{1/s}$, for which the calculation via the above formulae needs only $O(N^{1+1/s})$ operations. On the other hand, the rank-1 rule (1.3) with $n_1 = N$ and N prime requires $O(N^2)$ operations for the calculation of R by the above formulae.

In §2 we shall obtain an asymptotic series which can be used to approximate F_N. An error analysis of this asymptotic series is given in §3. We shall see that the function $F_N(x)$ can be accurately approximated for x sufficiently far away from 0, allowing R to be calculated in $O(N)$ operations.

From [14], P_α and R satisfy

$$P_\alpha \le (1+2\zeta(\alpha)N^{-\alpha})^s - 1 + (1+2\zeta(\alpha))^s R^\alpha. \tag{1.6}$$

Thus, it is possible to calculate bounds on P_α by first calculating R, and then using (1.6). In §4, such bounds on P_2 are obtained for some $s = 7$ rank-1 rules. The results given there indicate that the bounds on P_α obtained by using (1.6) are very poor. Much better bounds on P_α for rank-1 lattice rules may be found in [1] and [2], while [3] and [8] contain bounds on P_α for certain lattice rules of higher rank.

Besides calculating R explicitly, one may also be interested in theoretical bounds on R. Bounds on R for rank-1 lattice rules may be found in [13], while bounds for rank-2 lattice rules (but without explicit values for the constants) are to be found in [14]. More recently, Joe [7] has obtained bounds on R for certain lattice rules with rank ranging from 1 to s inclusive.

The results of some numerical calculations are presented in §4.

2. An asymptotic series for F_N

As we saw in the last section, for a lattice rule Q with N quadrature points, R is just the quadrature error $R(Q) = Qf_N - 1$, where

$$f_N(\mathbf{x}) = \prod_{k=1}^{s} F_N(x_k), \tag{2.1}$$

and

$$F_N(x) = 1 + \sum_{h \in E^*(N)} \frac{e^{\imath 2\pi h x}}{|h|}, \qquad 0 \le x \le 1,$$

which can be written as

$$F_N(x) = \begin{cases} 1 + 2\sum_{h=1}^{\frac{N-1}{2}} \dfrac{\cos(2\pi h x)}{h}, & N \text{ odd}, \\ 1 + 2\sum_{h=1}^{\frac{N-2}{2}} \dfrac{\cos(2\pi h x)}{h} + \dfrac{e^{\imath\pi N x}}{N/2}, & N \text{ even}. \end{cases} \tag{2.2}$$

We want to be able to evaluate F_N efficiently. With the notation

$$S(x, \eta) = \sum_{h=1}^{\eta - 1} \frac{\cos(2\pi h x)}{h},$$

we have

$$F_N(x) = \begin{cases} 1 + 2S(x, \eta(N)), & N \text{ odd}, \\ 1 + 2S(x, \eta(N)) + \dfrac{e^{\imath\pi N x}}{N/2}, & N \text{ even}, \end{cases} \tag{2.3}$$

where

$$\eta(N) = \begin{cases} \dfrac{N+1}{2}, & N \text{ odd}, \\ \dfrac{N}{2}, & N \text{ even}. \end{cases} \tag{2.4}$$

Thus, F_N can be accurately approximated if we can approximate $S(x, \eta)$ accurately. Shortly, we shall see that $S(x, \eta)$ can be adequately approximated by an asymptotic series, provided η is large enough and x is not too close to 0.

Since $S(x, \eta) = S(1-x, \eta)$, we may assume that $0 \le x \le \frac{1}{2}$. On writing

$$H(x, \eta) = \sum_{h=\eta}^{\infty} \frac{\cos(2\pi h x)}{h},$$

we have, for $0 < x \le \frac{1}{2}$,

$$S(x, \eta) = \sum_{h=1}^{\infty} \frac{\cos(2\pi h x)}{h} - H(x, \eta) = -\log(2\sin(\pi x)) - H(x, \eta), \tag{2.5}$$

where the last step follows from [4, p. 38]. Thus, we can obtain $S(x, \eta)$ from $H(x, \eta)$. (Korobov [11, Chapter 3] also used this identity.) We emphasize that (2.5) is not valid for $x = 0$, so in this case we should evaluate F_N directly by using (2.2).

Writing

$$\frac{1}{h} = \int_0^{\infty} e^{-ht}\, dt,$$

we have

$$\begin{aligned} H(x, \eta) &= \sum_{h=\eta}^{\infty} \int_0^{\infty} e^{-ht}\, dt \cos(2\pi h x) = \int_0^{\infty} \sum_{h=\eta}^{\infty} e^{-ht} \cos(2\pi h x)\, dt \\ &= \Re\left(\int_0^{\infty} \sum_{h=\eta}^{\infty} e^{-h(t+\imath 2\pi x)}\, dt\right) = \Re\left(\int_0^{\infty} \frac{e^{-\eta(t+\imath 2\pi x)}}{1-e^{-(t+\imath 2\pi x)}}\, dt\right) \\ &= \Re\left(e^{-\imath 2\pi(\eta-1)x} \int_0^{\infty} \frac{e^{-\eta t}}{e^{\imath 2\pi x} - e^{-t}}\, dt\right). \end{aligned}$$

Substitution of $w = e^{-t}$ into this last integral yields

$$H(x, \eta) = \Re(e^{-\imath 2\pi(\eta-1)x} G(x, \eta)), \tag{2.6}$$

where

$$G(x, \eta) = \int_0^1 \frac{w^{\eta-1}}{e^{\imath 2\pi x} - w}\, dw. \tag{2.7}$$

Once $G(x, \eta)$ is known, we may obtain the required function $H(x, \eta)$ from (2.6).

We now derive an asymptotic expansion which can be used to approximate $G(x, \eta)$ for $0 < x \le \frac{1}{2}$, provided η is large enough.

Theorem 2. *Suppose $G(x, \eta)$ is given by* (2.7). *Then for $0 < x \le \frac{1}{2}$*

$$G(x, \eta) \sim \sum_{k=0}^{\infty} \frac{(-1)^k k!}{\eta(\eta+1)\cdots(\eta+k)(e^{\imath 2\pi x} - 1)^{k+1}}.$$

Proof. We have

$$\begin{aligned}\frac{1}{e^{\imath 2\pi x}-w} &= \frac{1}{e^{\imath 2\pi x}-1}\times\frac{e^{\imath 2\pi x}-1}{e^{\imath 2\pi x}-w} = \frac{1}{e^{\imath 2\pi x}-1}\times\frac{e^{\imath 2\pi x}-1}{e^{\imath 2\pi x}-1-(w-1)}\\ &= \frac{1}{e^{\imath 2\pi x}-1}\times\frac{1}{1-\dfrac{w-1}{e^{\imath 2\pi x}-1}} = \frac{1}{e^{\imath 2\pi x}-1}\sum_{k=0}^{\infty}\frac{(w-1)^k}{(e^{\imath 2\pi x}-1)^k}\\ &= \sum_{k=0}^{\infty}\frac{(w-1)^k}{(e^{\imath 2\pi x}-1)^{k+1}},\end{aligned}$$

with the penultimate step holding if $|w-1|<|e^{\imath 2\pi x}-1|$. Then from (2.7) we obtain, by a formal term-by-term integration,

$$\begin{aligned}G(x,\eta) &\sim \int_0^1 w^{\eta-1}\sum_{k=0}^{\infty}\frac{(w-1)^k}{(e^{\imath 2\pi x}-1)^{k+1}}\,dw \sim \sum_{k=0}^{\infty}\frac{(-1)^k\int_0^1 w^{\eta-1}(1-w)^k\,dw}{(e^{\imath 2\pi x}-1)^{k+1}}\\ &= \sum_{k=0}^{\infty}\frac{(-1)^k\mathrm{B}(\eta,k+1)}{(e^{\imath 2\pi x}-1)^{k+1}} = \sum_{k=0}^{\infty}\frac{(-1)^k\Gamma(\eta)\Gamma(k+1)}{(e^{\imath 2\pi x}-1)^{k+1}\Gamma(\eta+k+1)}\\ &= \sum_{k=0}^{\infty}\frac{(-1)^k k!}{\eta(\eta+1)\cdots(\eta+k)(e^{\imath 2\pi x}-1)^{k+1}}.\end{aligned}$$

Thus far, the argument is purely formal. It remains to be shown that the series provides a valid asymptotic expansion of $G(x,\eta)$. For convenience, let us write the above series as

$$\sum_{k=0}^{\infty} a_k(x,\eta),$$

where

$$a_k(x,\eta) = \frac{(-1)^k k!}{\eta(\eta+1)\cdots(\eta+k)(e^{\imath 2\pi x}-1)^{k+1}}, \qquad k\ge 0. \tag{2.8}$$

Also, let $G_T(x,\eta)$ be the approximation to $G(x,\eta)$ obtained by truncating the series to $T+1$ terms, that is

$$G_T(x,\eta) = \sum_{k=0}^{T}\frac{(-1)^k k!}{\eta(\eta+1)\cdots(\eta+k)(e^{\imath 2\pi x}-1)^{k+1}} = \sum_{k=0}^{T} a_k(x,\eta). \tag{2.9}$$

Later we shall show (see Theorem 3) that

$$|G(x,\eta)-G_T(x,\eta)| \le 2|a_{T+1}(x,\eta)|. \tag{2.10}$$

That is, the error arising from truncating the series to $T+1$ terms is within a constant factor of the first omitted term, which can in turn be made arbitrarily small, for fixed x and T, by taking η large enough. The series is therefore a valid asymptotic expansion of $G(x,\eta)$ with respect to η, and the theorem is proved, subject to the need to prove (2.10). □

The asymptotic expansion for $G(x,\eta)$ given by Theorem 2 has complex terms. Since the desired function $H(x,\eta)$ is real, we would expect to be able to obtain it without using complex arithmetic. On using (2.6) and

$$e^{\imath 2\pi x}-1 = 2\imath e^{\imath\pi x}\sin(\pi x), \tag{2.11}$$

it can easily be shown that

$$H(x, \eta) \sim \sum_{k=0}^{\infty} \frac{(-1)^k k!}{\eta(\eta+1)\cdots(\eta+k)(2|\sin(\pi x)|)^{k+1}} \cdot \cos(2\pi(\eta-1)x + (k+1)\theta_x), \tag{2.12}$$

where $\theta_x = \arg(2\imath e^{\imath\pi x}\sin(\pi x)) = \pi\left(x + \frac{1}{2}\right)$. Thus we have an asymptotic expansion for $H(x, \eta)$ which involves only real terms. Upon substituting $\theta_x = \pi\left(x + \frac{1}{2}\right)$, we see that the asymptotic expansion in (2.12) can be written as

$$\sum_{k=0}^{\infty} b_k(x, \eta)\cos(\pi[(2\eta + k - 1)x + (k+1)/2]),$$

where $b_0(x, \eta) = 1/(2\eta|\sin(\pi x)|)$ and

$$\begin{aligned} b_{k+1}(x, \eta) &= \frac{(-1)^{k+1}(k+1)!}{\eta(\eta+1)\cdots(\eta+k+1)(2|\sin(\pi x)|)^{k+2}} \\ &= \frac{-(k+1)}{(\eta+k+1)2|\sin(\pi x)|} b_k(x, \eta). \end{aligned} \tag{2.13}$$

Thus, the $b_k(x, \eta)$ may be obtained recursively.

In practice, one must truncate the asymptotic expansion. With $G_T(x, \eta)$ defined by (2.9), let $H_T(x, \eta)$ be the corresponding truncation of (2.12), namely

$$\begin{aligned} H_T(x, \eta) &= \Re(e^{-\imath 2\pi(\eta-1)x} G_T(x, \eta)) \\ &= \sum_{k=0}^{T} b_k(x, \eta)\cos(\pi[(2\eta + k - 1)x + (k+1)/2]). \end{aligned} \tag{2.14}$$

Then we see from (2.3) and (2.5) that an approximation to F_N is given by $F_{N,T}$, where

$$F_{N,T}(x) = \begin{cases} 1 - 2\log(2|\sin(\pi x)|) - 2H_T(x, \eta(N)), & N \text{ odd}, \\ 1 - 2\log(2|\sin(\pi x)|) - 2H_T(x, \eta(N)) + \dfrac{e^{\imath\pi N x}}{N/2}, & N \text{ even}. \end{cases} \tag{2.15}$$

3. Error analysis and calculation of R

Before we can make effective use of the approximation to F_N given in (2.15), we need an error expression, so that we can make an appropriate choice of the truncation parameter T. This is the purpose of this section.

We see from (2.3), (2.5) and (2.15) that for $0 < x \le \frac{1}{2}$ we have

$$|F_N(x) - F_{N,T}(x)| = 2|H(x, \eta(N)) - H_T(x, \eta(N))|.$$

Moreover, it follows from (2.6) and (2.14) that

$$|H(x, \eta) - H_T(x, \eta)| \le |G(x, \eta) - G_T(x, \eta)|.$$

Thus, we obtain

$$|F_N(x) - F_{N,T}(x)| \le 2|G(x, \eta(N)) - G_T(x, \eta(N))|, \tag{3.1}$$

and so an error bound for $|F_N - F_{N,T}|$ may be obtained from an error bound for the truncated asymptotic expansion of $G(x, \eta)$. The required result is given in the following theorem.

Theorem 3. *Suppose* $G(x, \eta)$ *and* $G_T(x, \eta)$ *are given by* (2.7) *and* (2.9), *respectively. Then*

$$|G(x, \eta) - G_T(x, \eta)| \le 2|a_{T+1}(x, \eta)|.$$

Proof. As in the proof of Theorem 2, we write

$$\frac{1}{e^{\imath 2\pi x} - w} = \frac{1}{e^{\imath 2\pi x} - 1} \times \frac{1}{1 - \dfrac{w-1}{e^{\imath 2\pi x} - 1}}.$$

Since

$$\frac{1}{1-t} = \sum_{k=0}^{T} t^k + \frac{t^{T+1}}{1-t},$$

we see from (2.7) that

$$G(x, \eta) = \int_0^1 \sum_{k=0}^{T} \frac{w^{\eta-1}(w-1)^k}{(e^{\imath 2\pi x} - 1)^{k+1}}\, dw + \int_0^1 \frac{w^{\eta-1}(w-1)^{T+1}}{(e^{\imath 2\pi x} - 1)^{T+2}\left(1 - \dfrac{w-1}{e^{\imath 2\pi x} - 1}\right)}\, dw.$$

The derivation in Theorem 2 shows that the first integral in the above expression is just $G_T(x, \eta)$, and hence

$$\begin{aligned} |G(x, \eta) - G_T(x, \eta)| &= \left| \int_0^1 \frac{w^{\eta-1}(w-1)^{T+1}}{(e^{\imath 2\pi x} - 1)^{T+2}\left(1 - \dfrac{w-1}{e^{\imath 2\pi x} - 1}\right)}\, dw \right| \\ &\le \int_0^1 \frac{w^{\eta-1}(1-w)^{T+1}}{|e^{\imath 2\pi x} - 1|^{T+2}}\, dw \sup_{\substack{0<x\le\frac12 \\ 0\le w\le 1}} \frac{1}{\left|1 - \dfrac{w-1}{e^{\imath 2\pi x} - 1}\right|} \\ &= \sup_{\substack{0<x\le\frac12 \\ 0\le w\le 1}} \frac{1}{\left|1 - \dfrac{w-1}{e^{\imath 2\pi x} - 1}\right|} |a_{T+1}(x, \eta)|. \end{aligned}$$

Now

$$\left|1 - \frac{w-1}{e^{\imath 2\pi x} - 1}\right| = \left|\frac{w+1}{2} + \imath \frac{w-1}{2}\cot(\pi x)\right| \ge \frac{w+1}{2} \ge \tfrac12 \quad \text{for } w \in [0, 1].$$

Thus, for $w \in [0, 1]$ and $x \in \left(0, \frac12\right]$, we have

$$\frac{1}{\left|1 - \dfrac{w-1}{e^{\imath 2\pi x} - 1}\right|} \le 2,$$

and hence

$$|G(x, \eta) - G_T(x, \eta)| \le 2|a_{T+1}(x, \eta)|,$$

which completes the proof. □

We remark that a sharper result is possible in which the constant in the bound is not 2, but is a smaller number which depends on x.

From (3.1) and Theorem 3 we have

$$|F_N(x) - F_{N,T}(x)| \le 4|a_{T+1}(x, \eta(N))|.$$

This gives us an error expression involving the terms of the asymptotic expansion of $G(x, \eta)$. Now we see from (2.8), (2.11), and (2.13) that

$$|b_{T+1}(x, \eta)| = |a_{T+1}(x, \eta)|,$$

allowing us to write the above error expression as

$$|F_N(x) - F_{N,T}(x)| \le 4|b_{T+1}(x, \eta(N))|. \tag{3.2}$$

Thus, for given N and $\varepsilon > 0$, $F_{N,T}$ has an error of at most ε provided a T exists for which $4|b_{T+1}(x, \eta(N))| \le \varepsilon$. However, looking at the expression for $b_{T+1}(x, \eta)$ given by (2.13) we see that the error may be quite large for x close to 0 (we know already that we cannot use the expansion for $x = 0$), so we see that such a T does not always exist. In this case, F_N should be evaluated directly by using (2.2) rather than approximated by $F_{N,T}$. We now give a result which indicates, for given N, how far away x should be from 0 before we can obtain an accurate approximation to F_N. We shall see that for large enough x it may be arranged so that one needs at most about 14 terms to get an approximation accurate to about 10^{-15}.

Theorem 4. *Let $\varepsilon > 0$ and $N \ge 5$ be given. Suppose $F_N(x)$ is approximated by $F_{N,T}(x)$ for $\gamma/N \le x \le \frac{1}{2}$, where T and γ are positive integers satisfying*

$$2 \le \gamma \le \sqrt[3]{\frac{6N^2}{\pi^2}} \tag{3.3}$$

and

$$\frac{4(T+1)!}{(\gamma-1)^{T+2}\pi^{T+2}} \le \varepsilon. \tag{3.4}$$

Then

$$|F_N - F_{N,T}| \le \varepsilon.$$

Proof. Since

$$\sqrt[3]{\frac{6N^2}{\pi^2}} < \frac{N}{2} \quad \text{for } N \ge 5,$$

the assumption (3.3) implies $\gamma/N < \frac{1}{2}$. Now for $\gamma/N \le x \le \frac{1}{2}$,

$$2|\sin(\pi x)| \ge 2\left|\sin\left(\frac{\gamma\pi}{N}\right)\right| \ge 2\left[\frac{\gamma\pi}{N} - \frac{1}{6}\left(\frac{\gamma\pi}{N}\right)^3\right] \ge 2\frac{(\gamma-1)\pi}{N}, \tag{3.5}$$

provided

$$\frac{1}{6}\left(\frac{\gamma\pi}{N}\right)^3 \le \frac{\pi}{N},$$

which is equivalent to

$$\gamma \le \sqrt[3]{\frac{6N^2}{\pi^2}},$$

ensured by (3.3).

From (3.2) and (2.13) we have

$$\begin{aligned}|F_N(x) - F_{N,T}(x)| &\le \frac{4(T+1)!}{(2|\sin(\pi x)|)^{T+2}\eta(\eta+1)\cdots(\eta+T+1)} \\ &\le 4\left(\frac{N}{2(\gamma-1)\pi}\right)^{T+2}\frac{(T+1)!}{\eta(\eta+1)\cdots(\eta+T+1)},\end{aligned}$$

where the last step follows from (3.5). Now we note from (2.4) that $\eta = \eta(N) \geq N/2$ and hence

$$\frac{1}{\eta(\eta+1)\cdots(\eta+T+1)} \leq \frac{1}{\frac{N}{2}\left(\frac{N}{2}+1\right)\cdots\left(\frac{N}{2}+T+1\right)} \leq \frac{1}{\left(\frac{N}{2}\right)^{T+2}}.$$

Thus, we obtain

$$|F_N(x) - F_{N,T}(x)| \leq 4\left(\frac{N}{2(\gamma-1)\pi}\right)^{T+2} \frac{(T+1)!}{\left(\frac{N}{2}\right)^{T+2}} = \frac{4(T+1)!}{(\gamma-1)^{T+2}\pi^{T+2}} \leq \varepsilon,$$

using in the last step the assumption (3.4). □

In practice, we may apply the theorem with a fixed value of γ. For example, if we are content to restrict attention to $N \geq 115$, then we can satisfy (3.3) with $\gamma = 20$. For this value of γ one may easily verify that (3.4) is an equality if $T = 13$ and $\varepsilon = 8.0 \times 10^{-16}$. We have found this set of parameters to be a convenient choice for practical calculations.

Summarizing, to calculate R for an N-point lattice rule Q, we use $R(Q) = Qf_N - 1$, where, as we see from (2.1), f_N is just the product of 1-dimensional functions F_N. For $\gamma/N \leq x \leq \frac{1}{2}$ we can approximate $F_N(x)$ by the function $F_{N,T}(x)$ given by (2.15), where the function $H_T(x, \eta)$ in (2.15) is given by (2.14). For $0 \leq x < \gamma/N$ the explicit formula (2.2) is used. For $\frac{1}{2} < x \leq 1$ we can use the symmetry property of F_N: from (2.2) we have $F_N(x) = \overline{F_N(1-x)}$.

Used in this way, the explicit formula (2.2), which has of order $O(N)$ terms, needs to be used at most γ times, since according to [17] each component of each abscissa of an N-point lattice rule is an integer multiple of $1/N$. On the other hand, the approximation $F_{N,T}(x)$ needs to be used at most $N/2 - \gamma + 1$ times. Our operation count is based on the assumption that γ and T are fixed; for example, as noted above, the values $\gamma = 20$ and $T = 13$ give F_N with an absolute accuracy of 8.0×10^{-16} for all $N \geq 115$. Under this assumption, the explicit and asymptotic calculations each require $O(N)$ operations, and therefore so does the whole calculation.

4. Numerical results

Here we use the method described in the previous section to calculate R for some lattice rules of the rank-1 form (1.3). The parameter γ was taken to be 20. From the discussion at the end of the previous section, we know that for $\gamma/N \leq x \leq \frac{1}{2}$ and $N \geq 115$, $F_{N,T}(x)$ will have an error of at most $\varepsilon = 8.0 \times 10^{-16}$ if we take $T = 13$. However, it is not always necessary to take T as large as 13. From (3.2), we see that $F_{N,T}$ will have the desired accuracy if T is chosen to be the smallest integer for which $4|b_{T+1}(x, \eta(N))| \leq \varepsilon$. This was the procedure adopted in these calculations. For N odd, we can calculate R for the rank-1 rules (1.3) if we have the values of $F_N(x)$ or $F_{N,T}(x)$ at $x = 0, 1/N, \ldots, (N-1)/2N$. To save computation time, for a given value of N these $(N+1)/2$ values were calculated once and then stored.

TABLE 1

N	a	R	Bound on R	Bound on P_2	P_2
15019	12439	85295.22	106038.60	1.945(14)	1.196
18101	17487	80549.19	99749.35	1.735(14)	1.052
24041	1833	73509.11	90512.30	1.445(14)	0.693
33139	7642	65879.01	80621.20	1.160(14)	0.497
46213	37900	58420.63	71071.92	9.125(13)	0.328
57091	35571	53949.35	65395.89	7.782(13)	0.249
71053	31874	49554.02	59852.89	6.566(13)	0.210
100063	39040	43167.71	51859.84	4.982(13)	0.141

TABLE 2

N	Cpu Time A (seconds)	Cpu Time B (seconds)
15019	20.7	2594.4
18101	24.7	3763.4
24041	32.7	6630.5

The values of R calculated here were for rank-1 rules in $s = 7$ dimensions. The vectors $\mathbf{z}$ required in (1.3) were taken from Table 5 in Maisonneuve [12]. All these vectors are of the one-parameter Korobov form

$$\mathbf{z}(a) = (1, a, a^2, \dots, a^{s-1}) \pmod N), \qquad 1 \le a < N.$$

These given values of a were obtained by finding the value which minimized P_2.

Niederreiter [13] has obtained upper bounds on R for rank-1 rules. For composite N (all the values of N used were composite), these bounds are given by

$$R \le \frac{1}{N}(1.4 + 2\log N)^s.$$

These bounds as well as the actual values of R are given in Table 1. These bounds on R exceed the actual values by only about 20%. Using (1.6) (with $\alpha = 2$) we can also obtain bounds on P_2. These bounds as well as the actual value of P_2 are also given in Table 1. As can be seen, the bounds on P_2 are quite poor, being more than 10^{14} times larger than the actual values.

All the calculations were done on a Sequent 'Symmetry' computer. In Table 2 (under the heading 'Cpu time A') we give the cpu time required to calculate each of the values of R given in the first three rows of Table 1. It can be seen that these times are of order $O(N)$. For purposes of comparison, we also give in Table 2 (under the heading 'Cpu Time B') the cpu time required to calculate R by using (2.2) directly to evaluate $F_N(x)$ at $x = 0, 1/N, \dots, (N-1)/2N$ (which are then stored). It can be seen that these times are of order $O(N^2)$, and also that they are clearly not competitive, even for these values of N. As a check, the values of R calculated in the latter way agreed with the values of R given in Table 1 to at least the 7 digits shown.

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