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Parameters for Integrating Periodic Functions of Several Variables

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Abstract. A number-theoretical method for numerical integration of periodic functions of several variables was developed some years ago. This paper presents lists of numerical parameters to be used in implementing that method. The parameters define quadrature formulas for functions of $2, 3, \ldots, 8$ variables; error bounds for those formulas are also tabulated. The derivation of the parameters and error bounds is described.

1. Introduction. About twenty years ago, N. M. Korobov and E. Hlawka discovered a remarkable family of formulas for numerical quadrature of periodic functions of several variables [13]–[15], [8], [9]. To fix our notation, let us suppose that the function to be integrated has period 1 in each of its variables. Let "s" denote the number of variables and let the integration region be the unit cube $[0, 1]^s$ —which we shall denote "G_s", following Korobov. The formulas then take the form

$$If = \int_{G_s} f \approx Q_N f = \frac{1}{N} \sum_{r=1}^{N} f\left(\frac{r}{N}\mathbf{a}\right), \tag{1}$$

where $\mathbf{a}$ $(= \mathbf{a}(N))$ is an s-vector of integers that lie in $[1, N]$. The accuracy of the formula apparently depends on number-theoretic properties of the set of the integers in $\mathbf{a}$. Korobov and Hlawka showed that, as N runs through the sequence of primes, it is possible to find vectors $\mathbf{a}(N)$ such that the quadrature error

$$R_N f \equiv If - Q_N f = O\left(N^{-\alpha} \log^{\beta} N\right) \tag{2}$$

(for some α and β) for integrands f belonging to certain smoothness classes which we shall define below; and that for those classes this convergence is much faster than that afforded by the iterated (or Cartesian product) trapezoid rule.

Korobov called such vectors $\mathbf{a}(N)$ (or their components) "optimal coefficients," and Hlawka called them (with a slightly more stringent definition) "good lattice points". The quadrature method has become known variously as the method of "good lattices" or of "parallelepipedal nets." The reason is that the quadrature nodes in (1) can all be referred to the cube G_s by reducing each component "modulo 1"—i.e. to its fractional part. (This uses the periodicity of the integrand in each variable.) The resulting N points in G_s turn out to be lattice points of a certain slanted lattice (see e.g. [7] for illustrations of the 2-dimensional case). Geometrical properties of these lattices are intimately related to the accuracy of the quadrature formulas.

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The proof of the existence of good lattice points was constructive, but the method indicated for finding them involved very large amounts of computation for the values of N and s that are of most interest for numerical integration. This, together with the restriction of the number of quadrature nodes to a prime number (though Korobov did show that a product of 2 distinct primes was also all right) inhibited the use of the method of good lattices. Some sets of good lattice points were calculated, however (see e.g. [11], [16], [19]). Recently, these have been successfully used in various applications, and the method is receiving attention from chemists and physicists [3], [4], [21].

Numerical evidence [16] and also theoretical evidence [22] suggested that the condition that N be prime is not necessary. In 1973, P. Keast showed the existence of good lattice points $\mathbf{a}(N)$ whenever N is square-free [12], and S. K. Zaremba [23] showed their existence for all sufficiently large N. In 1978, H. Niederreiter [17] showed that they exist for all N. Thus, it should be possible to provide $\mathbf{a}(N)$'s for sequences of values of N that are convenient for practical numerical quadrature. The present paper provides such sequences for dimensions $s = 2, 3, \ldots, 8$ and for $N = 2^2, 2^3, 2^4, \ldots, 2^{17}$, together with the intermediate values $N = 3 \cdot 2, 3 \cdot 2^2, \ldots, 3 \cdot 2^{15}$. The method of calculation is one that was originally suggested in [6].

A recent survey of the method of good lattices, with extensive references to the literature, is contained in Section 4 of [18].

2. Error Bounds and the Search for Good Lattice Points. Korobov [14, pp. 29–31 and 146–156] described essentially the following scheme for obtaining error bounds for the quadrature formulas under discussion: Since our integrands are periodic, we shall classify them in terms of the speed of convergence of their Fourier series—which is known to be connected with the smoothness of the function. For any real $\alpha > 1$, let E_s^α be the class of all functions f of s variables, of period 1 in each variable, whose Fourier series

$$\sum_{m_1, \ldots, m_s = -\infty}^{\infty} c(\mathbf{m}) e^{2\pi i \mathbf{m} \cdot \mathbf{x}} \tag{3}$$

converges to $f(\mathbf{x})$ and satisfies the condition

$$|c(\mathbf{m})| \leq K \cdot \left(\prod_{r=1}^{s} \max\{1, |m_r|\} \right)^{-\alpha} \tag{4}$$

for some constant $K = K(f)$. The particular function F_s^α defined by

$$F_s^\alpha(\mathbf{x}) = \sum_{m_1, \ldots, m_s = -\infty}^{\infty} \left(\prod_{r=1}^{s} \max\{1, |m_r|\} \right)^{-\alpha} e^{2\pi i \mathbf{m} \cdot \mathbf{x}} \tag{5}$$

turns out to be a kind of extremal function for the class E_s^α: for any formula of the form (1), and any $f \in E_s^\alpha$,

$$|R_N f| \leq K(f) |R_N F_s^\alpha| ; \tag{6}$$

and this bound is sharp.

The idea of "goodness" for a sequence of lattice points can be defined precisely, in terms of the F_s^α, as follows:

Definition. For $\alpha > 1$ a "good lattice point sequence" for E_s^α is a sequence of integral s-vectors

(6a) $$\mathbf{a}(N_1), \mathbf{a}(N_2), \ldots$$

—corresponding to an infinite sequence $N_1 < N_2 < N_3 < \cdots$ of positive integers—such that the quadrature errors

(7a) $$R_N F_s^\alpha \equiv \int_{G_s} F_s^\alpha - \frac{1}{N} \sum_{r=1}^{N} F_s^\alpha\Big(\frac{r}{n}\mathbf{a}(N)\Big), \qquad N = N_1, N_2, \ldots,$$

satisfy

(7b) $$|R_N F_s^\alpha| \leqslant C N^{-\alpha} \operatorname{Log}^\beta N$$

for some numbers C and β independent of N.

By (6), such a sequence then affords an error bound of the same form as in (7b) for any function f in E_s^α.

An important property of the Korobov and Hlawka lattice points is that they are good for E_s^α, in this sense, for all values of α simultaneously. (The constants C and β of (7b) will vary with α.) This makes it unnecessary, when calculating an integral, to seek a formula that is suited to the smoothness of the specific integrand—which may be unknown. The Korobov-Hlawka formulas will automatically use all the smoothness the integrand has, to provide rapid convergence.

Indeed it is the case that any s-dimensional lattice point sequence that is good for E_s^α for a single $\alpha > 1$ is good for all $\alpha > 1$ and is "optimal" or "good" in the senses of Korobov and Hlawka. (This follows from the proof of Theorem 23 of [14].) So to find good lattice points it is sufficient, for each s and N, to find an $\mathbf{a}(N)$ that minimizes $|R_N F_s^\alpha|$, for some single value of α. This is Korobov's basic method.

For $\alpha = 2$, F_s^α can be written in the closed form

(8) $$F_s^\alpha(\mathbf{x}) = \prod_{r=1}^{s} \big(1 + 2\pi^2\big(x_r^2 - x_r + 1/6\big)\big)$$

for $\mathbf{x} \in G_s$; for $\mathbf{x}$ outside G_s the value of F_s^α is determined by periodicity. This makes the calculation of $R_N F_s^2$ particularly convenient. But it is still not practicable to calculate it for all N^s possible lattice points $\mathbf{a}$, to find a minimizing one—if N is even moderately large, and s is greater than 1 or 2.

However, it turns out that good lattice points are not unique or rare, but are quite common. It follows from Korobov's existence proof, for example, that for prime values of N half or more of all the possible lattice points $\mathbf{a}$ can be used in good lattice point sequences. Niederreiter's proof for general N implies the same, for the special set of lattice points $\mathbf{a}$ all of whose components are relatively prime to N. These facts suggest a search procedure for finding good lattice points. For any given s and N, choose at random some number M of lattice points, all of whose components are prime to N. For each one, calculate the error coefficient $|R_N F_s^2|$; a point for which the calculated error coefficient is least is very likely to be a good lattice point. That is the calculation—with $M = 40$—whose results we report here, but with one difference. The lattice points $\mathbf{a} = (a_1, a_2, \ldots, a_s)$ that were tried were all of the form

(9) $$a_r = \text{the residue of } b^{r-1} \bmod N, \qquad r = 1, 2, \ldots, s.$$

For each s and N we used 40 odd integers b, chosen at random in $[3, N-3]$. Korobov showed [14, pp. 148–149] that most $\mathbf{a}$'s of the special form (9) can be used

for good lattice point sequences, when N is prime. The numerical evidence presented below indicates that they also work well for general N. These special **a**'s have the practical advantage that the resulting quadrature formula (1) is fully defined by the single integer b rather than by s integers.

(We also deviated in a minor way from the search procedure described above in that we did not specify, when N was divisible by 3, that the randomly chosen values of b must not be divisible by 3. So in fact some of the lattice points that were tried out did not have all their components relatively prime to N. Interestingly, some of those were nevertheless successful—giving the lowest value found for $|R_N F_s^2|$, for the particular N and s.)

3. The Parameters. Tables 1, 2,..., 7 present the parameters obtained for integration formulas of the form (1), for dimensions 2, 3,..., 8, respectively. In each table, the first column lists the values of N, the second the values of the integration parameter b of formula (9), and the next 3 columns list the error bound coefficients $|R_N F_s^\alpha|$ of (6), for $\alpha = 2$, 4, and 6, respectively. The numbers in parentheses indicate the powers of 10.

The calculations were done on the UNIVAC 1108 at the National Bureau of Standards, with the final error bound coefficients being calculated in double precision. Due to roundoffs, the calculated bounds were in error by quantities of the order of 10^{-17}. As a result, we state to only one significant figure those coefficients that are of the order of 10^{-16}, and those that are less than 10^{-17} are not reported at all. We have included error bound coefficients between 10^{-17} and 10^{-16}, stated to one significant figure, but those results are not reliable.

4. Practical Considerations. One of the most attractive features of quadrature by the good lattice point method is that the accuracy—as seen in the error bounds (2) and (7b)—appears to be almost independent of the dimensionality s. This contrasts sharply with what happens when multiple integrals are evaluated using Cartesian products of 1-dimensional quadrature rules. In that situation, the rate of convergence takes the form $N^{-\gamma/s}$, where γ is some number characteristic of the smoothness of the integrand and N is the number of times the integrand is to be evaluated (see pp. 488–489 of [5]). For example, the Cartesian product trapezoid rule applied to functions of E_s^α may give convergence no faster than $N^{-\alpha/s}$—that will happen, in fact, for the function F_s^α defined above. For $s \geq 2$ that is much poorer than the $N^{-\alpha}\log^\beta N$ of (7b). This is so attractive that ways have been sought to apply good lattice points to nonperiodic integrands. A simple one is as follows: For $s = 1$, replace the integrand $f(x)$ by the function $g(x) = (f(x) + f(1-x))/2$. The integral of g is equal to that of f, and g is somewhat periodic: $g(0) = g(1)$. For $s = 2$, use

$$g(x_1, x_2) = \tfrac{1}{4}\{f(x_1, x_2) + f(1-x_1, x_2) + f(x_1, 1-x_2) + f(1-x_1, 1-x_2)\},$$

with similar formulas in higher dimensions. These g's will belong to E_s^2, if the original integrand f is sufficiently smooth—a sufficient condition is that all mixed partial derivatives, that are of order 1 or less with respect to each variable, exist and are continuous on G_s. There are more complicated methods of "periodizing" integrands which can produce functions in E_s^α with $\alpha > 2$. They are discussed in [14, pp. 52–65], and in [10, pp. 121–130].

TABLE 1: $s = 2$

N	b	$\lvert R_N F_2^2 \rvert$	$\lvert R_N F_2^4 \rvert$	$\lvert R_N F_2^6 \rvert$
4	1	3.88 (0)	2.10 (0)	2.01 (0)
6	1	2.94 (0)	2.03 (0)	2.01 (0)
8	3	1.09 (0)	6.55 (-2)	6.26 (-3)
12	5	5.57 (-1)	1.66 (-2)	7.84 (-4)
16	7	3.73 (-1)	1.04 (-2)	5.31 (-4)
24	9	1.66 (-1)	1.34 (-3)	1.64 (-5)
32	9	1.24 (-1)	1.24 (-3)	2.11 (-5)
48	21	5.28 (-2)	1.60 (-4)	8.49 (-7)
64	27	3.16 (-2)	4.64 (-5)	1.05 (-7)
96	21	1.66 (-2)	1.74 (-5)	3.09 (-8)
128	29	9.53 (-3)	4.72 (-6)	4.17 (-9)
192	51	4.85 (-3)	1.33 (-6)	5.50 (-10)
256	99	2.49 (-3)	2.13 (-7)	2.71 (-11)
384	141	1.14 (-3)	3.95 (-8)	2.03 (-12)
512	189	7.22 (-4)	1.90 (-8)	7.76 (-13)
768	225	3.21 (-4)	3.12 (-9)	4.44 (-14)
1024	399	2.15 (-4)	1.95 (-9)	2.86 (-14)
1536	447	9.13 (-5)	2.66 (-10)	1.2 (-15)
2048	849	6.89 (-5)	3.54 (-10)	3.8 (-15)
3072	1273	2.53 (-5)	1.97 (-11)	4(?) (-17)
4096	1787	1.66 (-5)	1.11 (-11)	--
6144	2269	7.12 (-6)	1.69 (-12)	--
8192	3453	4.39 (-6)	8.56 (-13)	--
12288	5181	1.86 (-6)	1.04 (-13)	--
16384	6279	1.19 (-6)	5.45 (-14)	--
24576	7301	5.10 (-7)	7.6 (-15)	--
32768	5133	3.87 (-7)	8.7 (-15)	--
49152	6503	1.80 (-7)	1.8 (-15)	--
65536	27627	1.04 (-7)	6. (-16)	--
98304	29153	4.32 (-8)	6(?) (-17)	--
131072	34613	2.38 (-8)	2(?) (-17)	--

TABLE 2: $s = 3$

N	b	$\lvert R_N F_3^{2} \rvert$	$\lvert R_N F_3^{4} \rvert$	$\lvert R_N F_3^{6} \rvert$
4	1	1.88 (1)	7.09 (0)	6.22 (0)
6	1	1.34 (1)	6.50 (0)	6.10 (0)
8	3	8.57 (0)	2.57 (0)	2.11 (0)
12	3	5.54 (0)	2.16 (0)	2.02 (0)
16	5	3.51 (0)	3.44 (-1)	7.00 (-2)
24	3	1.92 (0)	9.64 (-2)	9.14 (-3)
32	11	1.42 (0)	6.65 (-2)	6.19 (-3)
48	9	7.21 (-1)	1.45 (-2)	6.26 (-4)
64	5	5.64 (-1)	1.08 (-2)	3.55 (-4)
96	39	2.85 (-1)	3.04 (-3)	6.52 (-5)
128	41	1.76 (-1)	7.11 (-4)	5.22 (-6)
192	39	9.17 (-2)	1.93 (-4)	6.92 (-7)
256	37	5.91 (-2)	8.85 (-5)	2.47 (-7)
384	81	2.78 (-2)	1.22 (-5)	9.33 (-9)
512	123	1.97 (-2)	8.80 (-6)	7.46 (-9)
768	75	9.69 (-3)	2.45 (-6)	1.38 (-9)
1024	173	6.69 (-3)	1.17 (-6)	3.92 (-10)
1536	375	3.41 (-3)	3.36 (-7)	6.68 (-11)
2048	753	2.04 (-3)	9.53 (-8)	8.55 (-12)
3072	1491	1.30 (-3)	1.22 (-7)	2.50 (-11)
4096	1271	8.85 (-4)	2.65 (-8)	1.31 (-12)
6144	1907	3.64 (-4)	3.46 (-9)	6.53 (-14)
8192	2835	2.11 (-4)	8.66 (-10)	6.6 (-15)
12288	2469	1.30 (-4)	7.29 (-10)	7.9 (-15)
16384	1163	8.00 (-5)	2.03 (-10)	1.2 (-15)
24576	7223	3.39 (-5)	2.89 (-11)	8(?) (-17)
32768	8655	2.06 (-5)	1.20 (-11)	2(?) (-17)
49152	14441	1.34 (-5)	6.88 (-12)	5(?) (-17)
65536	22201	5.93 (-6)	1.06 (-12)	--
98304	12525	2.93 (-6)	2.59 (-13)	--
131072	42445	2.35 (-6)	3.70 (-13)	--

TABLE 3: $s = 4$

N	b	$\lvert R_N F_4^{2} \rvert$	$\lvert R_N F_4^{4} \rvert$	$\lvert R_N F_4^{6} \rvert$
4	1	8.38 (1)	2.46 (1)	2.09 (1)
6	1	5.74 (1)	2.03 (1)	1.85 (1)
8	3	4.17 (1)	1.23 (1)	1.05 (1)
12	3	2.60 (1)	7.31 (0)	6.24 (0)
16	5	2.03 (1)	5.31 (0)	4.28 (0)
24	3	1.22 (1)	2.67 (0)	2.12 (0)
32	3	9.82 (0)	2.55 (0)	2.11 (0)
48	21	5.22 (0)	3.80 (-1)	7.30 (-2)
64	21	3.83 (0)	2.37 (-1)	4.10 (-2)
96	21	2.23 (0)	7.46 (-2)	6.38 (-3)
128	21	1.55 (0)	2.92 (-2)	1.32 (-3)
192	5	9.01 (-1)	1.32 (-2)	4.43 (-4)
256	39	6.14 (-1)	4.61 (-3)	8.09 (-5)
384	187	3.25 (-1)	1.06 (-3)	8.35 (-6)
512	107	2.53 (-1)	9.70 (-4)	7.71 (-6)
768	197	1.40 (-1)	2.96 (-4)	1.52 (-6)
1024	493	9.13 (-2)	1.10 (-4)	2.90 (-7)
1536	369	5.73 (-2)	8.96 (-5)	3.17 (-7)
2048	941	3.85 (-2)	2.49 (-5)	3.47 (-8)
3072	501	1.92 (-2)	4.72 (-6)	2.08 (-9)
4096	2023	1.32 (-2)	3.06 (-6)	1.39 (-9)
6144	2679	6.67 (-3)	1.15 (-6)	5.99 (-10)
8192	539	3.96 (-3)	1.88 (-7)	2.05 (-11)
12288	2187	2.53 (-3)	1.92 (-7)	3.74 (-11)
16384	2037	1.58 (-3)	4.35 (-8)	2.55 (-12)
24576	6833	8.19 (-4)	1.71 (-8)	9.00 (-13)
32768	11579	6.19 (-4)	1.54 (-8)	1.05 (-12)
49152	2999	2.88 (-4)	1.06 (-9)	8.2 (-15)
65536	18793	1.90 (-4)	5.42 (-10)	2.7 (-15)
98304	1497	1.15 (-4)	2.75 (-10)	1.2 (-15)
131072	2771	6.46 (-5)	1.32 (-10)	6 (-16)

TABLE 4: $s = 5$

N	b	$\lvert R_N F_5^2 \rvert$	$\lvert R_N F_5^4 \rvert$	$\lvert R_N F_5^6 \rvert$
4	1	3.63 (2)	7.85 (1)	6.36 (1)
6	1	2.45 (2)	6.04 (1)	5.20 (1)
8	3	1.81 (2)	3.92 (1)	3.18 (1)
12	3	1.15 (2)	2.53 (1)	2.10 (1)
16	5	8.99 (1)	1.88 (1)	1.50 (1)
24	3	5.72 (1)	1.26 (1)	1.05 (1)
32	5	4.34 (1)	6.82 (0)	4.58 (0)
48	21	2.80 (1)	5.47 (0)	4.29 (0)
64	13	2.02 (1)	1.50 (0)	3.09 (-1)
96	21	1.37 (1)	2.63 (0)	2.12 (0)
128	3	9.63 (0)	5.97 (-1)	1.12 (-1)
192	3	5.66 (0)	2.71 (-1)	4.39 (-2)
256	21	4.06 (0)	6.80 (-2)	2.73 (-3)
384	141	2.82 (0)	1.72 (-1)	3.49 (-2)
512	151	1.82 (0)	2.60 (-2)	1.16 (-3)
768	9	1.07 (0)	7.46 (-3)	1.31 (-4)
1024	363	7.35 (-1)	2.92 (-3)	3.04 (-5)
1536	297	5.01 (-1)	2.70 (-3)	3.04 (-5)
2048	659	3.04 (-1)	6.08 (-4)	2.93 (-6)
3072	1425	1.89 (-1)	5.50 (-4)	4.68 (-6)
4096	661	1.34 (-1)	1.74 (-4)	5.06 (-7)
6144	2291	7.48 (-2)	5.01 (-5)	8.01 (-8)
8192	3333	4.83 (-2)	2.34 (-5)	3.90 (-8)
12288	4999	3.08 (-2)	1.21 (-5)	1.41 (-8)
16384	2705	2.06 (-2)	4.44 (-6)	2.40 (-9)
24576	2453	1.20 (-2)	1.95 (-6)	1.04 (-9)
32768	145	8.81 (-3)	8.66 (-7)	1.77 (-10)
49152	1509	4.07 (-3)	1.61 (-7)	1.85 (-11)
65536	18351	3.04 (-3)	1.55 (-7)	2.00 (-11)
98304	24093	1.70 (-3)	6.76 (-8)	6.00 (-12)
131072	2771	1.09 (-3)	2.50 (-8)	1.70 (-12)

TABLE 5: $s = 6$

N	b	$\lvert R_N F_6^2 \rvert$	$\lvert R_N F_6^4 \rvert$	$\lvert R_N F_6^6 \rvert$
4	1	1.56 (3)	2.51 (2)	1.95 (2)
6	1	1.05 (3)	1.83 (2)	1.50 (2)
8	3	7.78 (2)	1.25 (2)	9.65 (1)
12	3	4.95 (2)	8.07 (1)	6.38 (1)
16	5	3.89 (2)	6.14 (1)	4.73 (1)
24	3	2.48 (2)	4.03 (1)	3.19 (1)
32	3	1.94 (2)	3.05 (1)	2.36 (1)
48	3	1.24 (2)	1.94 (1)	1.50 (1)
64	11	9.38 (1)	9.35 (0)	5.08 (0)
96	45	5.99 (1)	7.07 (0)	4.61 (0)
128	5	4.42 (1)	2.47 (0)	4.88 (-1)
192	51	2.86 (1)	1.64 (0)	3.21 (-1)
256	123	2.18 (1)	1.12 (0)	2.14 (-1)
384	141	1.40 (1)	6.77 (-1)	1.19 (-1)
512	3	9.64 (0)	3.42 (-1)	5.01 (-2)
768	9	6.25 (0)	2.23 (-1)	3.84 (-2)
1024	491	4.62 (0)	7.06 (-2)	3.43 (-3)
1536	341	2.80 (0)	2.82 (-2)	9.17 (-4)
2048	443	2.13 (0)	2.22 (-2)	7.97 (-4)
3072	1095	1.34 (0)	1.30 (-2)	5.43 (-4)
4096	1271	8.95 (-1)	2.70 (-3)	1.98 (-5)
6144	1477	5.33 (-1)	1.14 (-3)	6.56 (-6)
8192	67	3.56 (-1)	3.49 (-4)	8.37 (-7)
12288	5685	2.37 (-1)	3.63 (-4)	1.74 (-6)
16384	7011	1.62 (-1)	1.64 (-4)	5.32 (-7)
24576	3771	1.04 (-1)	1.12 (-4)	3.85 (-7)
32768	4335	6.71 (-2)	1.94 (-5)	1.39 (-8)
49152	1509	3.44 (-2)	5.83 (-6)	2.90 (-9)
65536	24565	2.95 (-2)	4.09 (-6)	1.31 (-9)
98304	40709	1.70 (-2)	2.44 (-6)	9.52 (-10)
131072	33269	1.40 (-2)	2.80 (-6)	1.61 (-9)

TABLE 6: $s = 7$

N	b	$\lvert R_N F_7^2 \rvert$	$\lvert R_N F_7^4 \rvert$	$\lvert R_N F_7^6 \rvert$
4	1	6.69 (3)	7.94 (2)	5.92 (2)
6	1	4.47 (3)	5.60 (2)	4.34 (2)
8	3	3.35 (3)	3.96 (2)	2.95 (2)
12	3	2.13 (3)	2.58 (2)	1.96 (2)
16	5	1.67 (3)	1.98 (2)	1.48 (2)
24	3	1.07 (3)	1.28 (2)	9.68 (1)
32	5	8.35 (2)	9.87 (1)	7.37 (1)
48	3	5.31 (2)	6.31 (1)	4.75 (1)
64	11	4.15 (2)	4.29 (1)	2.92 (1)
96	21	2.65 (2)	3.14 (1)	2.37 (1)
128	5	2.05 (2)	1.99 (1)	1.35 (1)
192	45	1.31 (2)	1.16 (1)	7.07 (0)
256	99	9.98 (1)	6.23 (0)	2.79 (0)
384	51	6.19 (1)	2.66 (0)	5.03 (-1)
512	93	4.91 (1)	2.24 (0)	4.28 (-1)
768	333	3.07 (1)	1.23 (0)	2.23 (-1)
1024	141	2.26 (1)	9.19 (-1)	1.95 (-1)
1536	297	1.41 (1)	3.15 (-1)	4.30 (-2)
2048	683	1.05 (1)	2.28 (-1)	2.07 (-2)
3072	39	7.05 (0)	1.29 (-1)	9.30 (-3)
4096	1159	5.08 (0)	4.64 (-2)	1.65 (-3)
6144	1731	3.32 (0)	4.77 (-2)	3.52 (-3)
8192	3091	2.38 (0)	1.10 (-2)	1.49 (-4)
12288	4611	1.38 (0)	4.65 (-3)	4.99 (-5)
16384	2037	1.14 (0)	1.00 (-2)	5.04 (-4)
24576	4059	6.97 (-1)	3.19 (-3)	5.75 (-5)
32768	453	4.58 (-1)	6.27 (-4)	3.32 (-6)
49152	12295	3.10 (-1)	5.83 (-4)	4.87 (-6)
65536	4855	1.94 (-1)	1.37 (-4)	3.64 (-7)
98304	237	1.35 (-1)	1.24 (-4)	4.01 (-7)
131072	33269	9.27 (-2)	5.32 (-5)	1.37 (-7)

TABLE 7: $s = 8$

N	b	$\lvert R_N F_8^{2} \rvert$	$\lvert R_N F_8^{4} \rvert$	$\lvert R_N F_8^{6} \rvert$
4	1	2.87 (4)	2.52 (3)	1.80 (3)
6	1	1.92 (4)	1.74 (3)	1.28 (3)
8	3	1.44 (4)	1.26 (3)	8.99 (2)
12	3	9.13 (3)	8.16 (2)	5.94 (2)
16	5	7.17 (3)	6.29 (2)	4.50 (2)
24	3	4.57 (3)	4.07 (2)	2.96 (2)
32	5	3.59 (3)	3.14 (2)	2.24 (2)
48	21	2.29 (3)	2.04 (2)	1.48 (2)
64	11	1.79 (3)	1.51 (2)	1.05 (2)
96	21	1.14 (3)	1.02 (2)	7.39 (1)
128	35	8.95 (2)	7.59 (1)	5.31 (1)
192	51	5.68 (2)	4.72 (1)	3.31 (1)
256	99	4.44 (2)	3.39 (1)	2.25 (1)
384	51	2.80 (2)	2.05 (1)	1.36 (1)
512	93	2.17 (2)	1.29 (1)	7.26 (0)
768	237	1.37 (2)	4.75 (0)	8.69 (-1)
1024	141	1.03 (2)	4.86 (0)	2.54 (0)
1536	291	6.83 (1)	2.34 (0)	4.30 (-1)
2048	443	5.04 (1)	1.42 (0)	2.69 (-1)
3072	1229	3.31 (1)	8.36 (-1)	1.43 (-1)
4096	595	2.54 (1)	6.66 (-1)	1.13 (-1)
6144	1923	1.62 (1)	3.40 (-1)	4.56 (-2)
8192	2153	1.15 (1)	1.07 (-1)	4.98 (-3)
12288	4251	7.56 (0)	5.59 (-2)	1.57 (-3)
16384	6957	5.64 (0)	3.15 (-2)	8.87 (-4)
24576	10517	3.85 (0)	2.45 (-2)	5.62 (-4)
32768	453	2.45 (0)	5.56 (-3)	5.31 (-5)
49152	1509	1.73 (0)	8.68 (-3)	1.62 (-4)
65536	25219	1.21 (0)	3.01 (-3)	3.20 (-5)
98304	40709	7.54 (-1)	8.33 (-4)	2.98 (-6)
131072	11495	5.87 (-1)	1.21 (-3)	1.13 (-5)

However, looking through the tables quickly shows that the error bound coefficients $|R_N F_s^\alpha|$ are not entirely independent of s. Focusing on $\alpha = 2$, we see that $|R_{1024} F_s^2|$ grows rapidly with s: from .000215 for $s = 2$, through .00669, .0913, .735, 4.62, 22.6, to 103 for $s = 8$. This is partly due to the dependence on s of the exponent β in the error bound in (7b); the nature of this dependence is not entirely known, and will be discussed below. The constant C in (7b) may also depend on s—the numerical evidence suggests that it decreases as s increases.

With Cartesian product formulas it seems, from the convergence rate $N^{-\gamma/s}$, that the computational effort (measured by the value of N) that is needed to achieve a given level of accuracy will rise exponentially as s increases. To get an idea of what happens in the method of good lattice points, we may fix $\alpha = 2$, for example, and look, for each s, at the value of N that brings $|R_N F_s^2|$ down to a prescribed level—say 0.1 (This is of course not the same as asking what value of N will give an absolute error, or relative error, of 0.1 for any particular integrand of interest—other than F_s^2 itself.) The results we obtain, by interpolating very roughly in Tables 1–7,

s	2	3	4	5	6	7	
N	35	180	900	5,000	25,000	125,000	

Similar results are obtained when 0.1 is replaced by some other number—1.0, or 0.01. It seems that for the function classes E_s^2, the N required for any given level of accuracy does increase with s, roughly as fast as 5^s, when the formulas of the present paper are used. For E_s^4, a similar calculation indicates that the increase is roughly as 2.5^s.

So the good lattice point method does not entirely overcome the "curse of dimensionality". But it does mitigate it. To compare, if the trapezoid rule were to require N_0 evaluation points to integrate F_1^2 to some given level of accuracy—and N_0 might be 2, or 10, or 100, then the Cartesian product trapezoid rule would require N_0^s to evaluate F_s^2 to similar accuracy. In contrast, the 5^s growth rate for the good lattice point formulas is roughly independent of the level of accuracy.

5. Discussion. There is another method for obtaining lattice points that may be "good" in the sense discussed here, and that does not require even as much calculation as does our random search. That is the method of L. K. Hua and Y. Wang, which is based on concepts of algebraic number theory and diophantine approximation. A full exposition can be found in [10], and a short description in Section 2 of [6]. It is not known whether this method actually produces good lattice points, but the numerical evidence suggests that it does. A number of lattice points have been calculated by this method, together with corresponding error bound coefficients; see Tables I–III of [6], and the entries marked by asterisks in Tables 1–12 (pp. 224–234) of [10]. A comparison of the values of $|R_N F_s^2|$ given there (called "B" in [6], and "$W_2(n, h)$" in [10]) with those given in the tables above indicates that for $s = 3$, 4, and 5 the quadrature formulas obtained by the method of Hua and Wang have considerably larger error bound coefficients than those produced by the random search method. However, for $s = 6$ and 7, the error bound coefficients obtained by the two methods are fairly close. (This is perhaps best seen when the coefficients are plotted in the manner of Figure 1 below.) The Hua-Wang method is restricted to certain sequences of values of N.

One important piece of information, that has not yet been provided by the theoretical developments, is the best possible value of β in the error estimate (7b). Calling this lowest β (or the inf of all such β) "β^*", we might expect that β^* will be a function of α and s in general. Indeed Korobov and Hlawka (see e.g. [14, pp. 95–102]) showed that $\beta^* \leqslant s\alpha$, and N. S. Bahvalov [1] improved this to $\beta^* \leqslant (s-1)\alpha$. In the opposite direction, all that is known is that $\beta^* \geqslant s-1$ for all $\alpha > 1$ [20]. The only definitive result is that, for $s = 2$, $\beta^* = 1$ independently of α [1].

Thus it is interesting to see what values of β are indicated by the numerical results presented above. Figure 1 shows the result of plotting $\log(N^2 \mid R_N F_s^2 \mid)$ versus $\log(\log(N))$ for the calculated values of $R_N F_s^2$. (Only those values with $\mid R_N F_s^2 \mid < 10$ were included in the graph. Examination of the tables above shows that convergence faster than $O(1/N)$ does not begin to be apparent until the error bound coefficient drops to between 10 and 1; the higher values (for lower N) are controlled by factors different from those determining the asymptotic convergence rate.) The points group themselves naturally into seven approximate lines, depending on the dimension number s; $s = 2$ is at the bottom, $s = 8$ at the top.

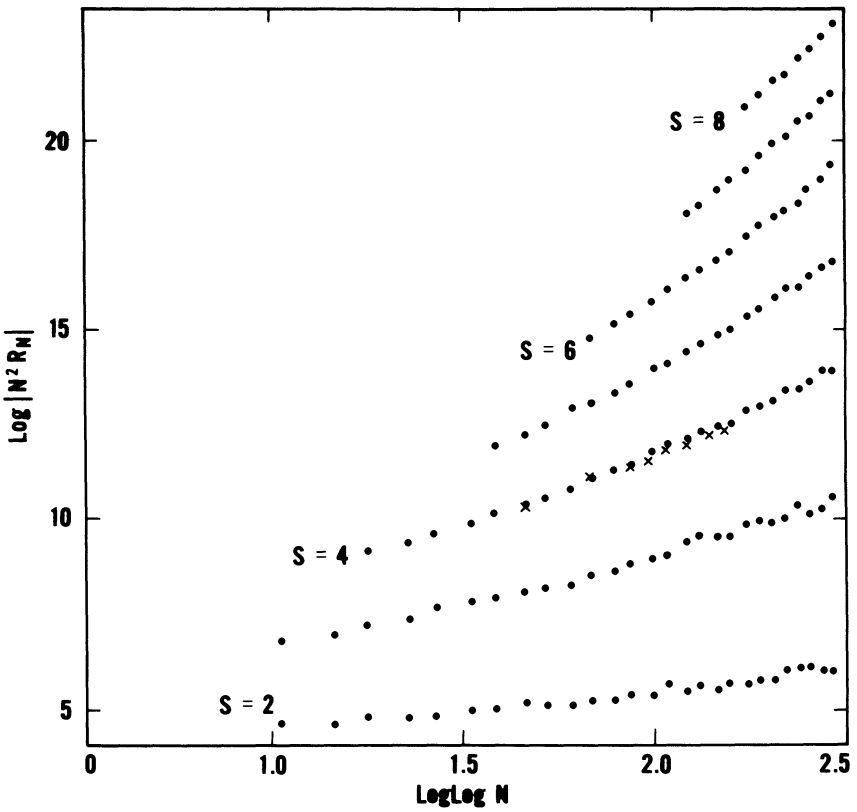

FIGURE 1

An asymptotic relation of the form

$$|R_N F_s^2| \sim C(s) N^{-2} \log \beta(s) N$$

(for the lattice points obtained) would result in each group of points being asymptotic to a straight line of slope $\beta(s)$. Some irregularity is to be expected: the random search by which the lattice points were obtained causes some statistical irregularity in their quality, and the number-theoretical nature of the error bound also suggests that it will not behave smoothly.

Table 8 gives the approximate slopes, for each s, that I obtained by a rough visual fit of a straight line to each group of points (no more refined procedure seems justified).

TABLE 8

s	2	3	4	5	6	7	8
$\beta(s)$	1.2	2.8	4.3	5.8	6.9	8.3	9.6

These values are definitely lower than the $2(s-1)$ that is the best that we can be sure—by theory—is obtainable; they are also higher than Sarygin's lower bound of $s-1$.

The x's appearing in Figure 1 represent a set of error bound coefficients obtained by a different method. In that calculation, the N's investigated were prime, so that good lattice points of the form (9) must exist. I obtained the best possible ones by exhaustive calculation of $|R_N F_s^2|$ for all such lattice points. This lengthy calculation was done for $s = 4$; the highest N was 7001. The results suggest that the random search procedure yields quadrature formulas that are very nearly as accurate as those obtained by exhaustive search, and that convenient nonprime values of N are just as useable, for this method of integration, as primes.

(*Remark*. Having several hundred error-bound coefficients in a computer file suggested looking at the relative frequencies of their lead digits. They are

lead digit	1	2	3	4	5	6	7	8	9
number of occurrences	185	127	74	57	52	47	34	33	27
relative frequency	.291	.200	.116	.090	.082	.074	.053	.052	.042

This agrees well with Benford's "Law of Anomalous Numbers" [2].)

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