

A Modified Monte-Carlo Quadrature. II*

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1. Introduction. In a previous paper ("A modified Monte-Carlo quadrature," *Math. Comp.*, v. 19, 1966, pp. 361-368; I shall refer to it below as "MMC") I proposed a Monte-Carlo quadrature procedure which incorporated a very simple form of stratified sampling and which produces somewhat more accurate estimates of integrals than would be obtained by simple Monte-Carlo. As applied to integration over the s -dimensional unit cube G_s (i.e., G_s is the set of all $x = (x^1, x^2, \dots, x^s)$ such that $0 \leq x^i \leq 1$ for $i = 1, \dots, s$) the method was as follows: Let n_1, n_2, \dots, n_s be positive integers, and partition G_s into $N = n_1 \cdot n_2 \cdot \dots \cdot n_s$ congruent subintervals by dividing the interval $[0,1]$ on the x^i -axis, for each i , into n_i equal subintervals. Choose one point at random in each of these N parts of G_s , and call those points—in any order— x_1, x_2, \dots, x_N ; then take the quantity

$$(1) \quad \frac{1}{N} \sum_{r=1}^N f(x_r)$$

as the estimate of the integral over G_s of the function f .

In the simplest case the numbers n_1, n_2, \dots, n_s are all taken equal so that G_s is partitioned into N subcubes and $N = K^s$ for some positive integer K . The present paper proposes a second modification of simple Monte-Carlo quadrature, which makes further use of this partition of G_s .

If N is large, so that each of the subcubes into which G_s is divided is quite small one would generally suppose that the integrand would be a monotonic function of each x^i in most of the subcubes. Thinking along the lines of Hammersley and Morton's method of antithetic variates [1], [2], it would seem that if x is a point chosen at random in a subcube and x' is the point symmetrically opposite it in that subcube, the quantity

$$(f(x) + f(x'))/2$$

should have smaller variance than $f(x)$. We therefore define the following estimate for $\int_G f$: Dividing G_s into $N = K^s$ subcubes as above, call these subcubes, in some order, A_1, A_2, \dots, A_N . For $1 \leq r \leq N$, let c_r be the center of A_r , and choose a single point—call it x_r —at random in A_r ; and let $x_r' = 2c_r - x_r$. Then our estimate is

$$(2) \quad J_2 = J_2(f, N) = \frac{1}{N} \sum_{r=1}^N \frac{f(x_r) + f(x_r')}{2}.$$

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(The quantity (1) we shall denote by J_1 , while “ J_0 ” will designate the simple Monte-Carlo estimate

$$(3) \quad \frac{1}{N} \sum_{r=1}^N f(y_r)$$

where the N points y_r are chosen at random in G_s .)

2. Error Analysis. The discussion of the error of these estimates is based on the usual assumption of Monte-Carlo theory, that the points y_r and the points x_r can be regarded as independent (or at least pairwise independent) random variables; in our case each y_r is uniformly distributed over G_s , while x_r is uniformly distributed over A_r . Then J_0, J_1 , and J_2 are random variables, and it is easy to see that all three have the integral of f as mean value:

$$(4) \quad m(J_i) = I = \int_{G_s} f, \quad i = 0, 1, 2.$$

(For J_2 we note that x_r' is, like x_r , uniformly distributed over A_r ; so that

$$m(J_2) = \frac{1}{N} \sum_{r=1}^N \frac{1}{2} (m(f(x_r)) + m(f(x_r'))) = \frac{1}{N} \sum_{r=1}^N N \int_{A_r} f = I.)$$

Numerical evaluation of an integral by the formula (1), (2), or (3) then can be regarded as taking a sample value of one of the J 's as an estimate of the mean I ; so that the standard deviation of that J may be taken as a measure of the error to be expected. On the usual assumption that J is approximately normally distributed, there would then be a probability of 1/2 that the error of the estimate is less than about (5/8) $\sigma(J)$, while the chance that the error is greater than $2\sigma(J)$ would be less than 1/20.

We set

$$(5) \quad \sigma_N(J_0) = \sigma(J_0(f, N)), \quad \sigma_N(J_1) = \sigma(J_1(f, N)), \quad \sigma_{2N}(J_2) = \sigma(J_2(f, N)),$$

so that the subscript of σ is equal, in each case, to the number of evaluations of the integrand required for the estimate of I . For the simple Monte-Carlo estimator J_0 we have the well-known result:

$$(6) \quad \sigma_N(J_0) = d_0 N^{-1/2}, \quad d_0^2 = \int_{G_s} f^2 - \left(\int_{G_s} f \right)^2.$$

In MMC I showed that $\sigma_N(J_1) \leq \sigma_N(J_0)$ for any $f \in L^2(G_s)$; for continuous f , $\sigma_N(J_1)/\sigma_N(J_0) \rightarrow 0$ as $N \rightarrow \infty$; and if the gradient ∇f exists and is continuous on G_s , then

$$(7) \quad \sigma_N(J_1) = d_1 N^{-(1/2+1/s)} + o(N^{-(1/2+1/s)}), \quad d_1 = \left(\int_{G_s} |\nabla f|^2 \right)^{1/2}.$$

The first of these three results has no analogue for J_2 —it may happen that $\sigma_{2N}(J_2) > \sigma_{2N}(J_0)$. However, for smooth integrands we have the following:

THEOREM. *If $\partial^2 f / \partial x^i \partial x^j$ is continuous on G_s for $1 \leq i, j \leq s$, then*

$$(8) \quad \sigma_{2N}(J_2) = (d_2 + o(1)) N^{-(1/2+2/s)}$$

where

$$(8') \quad d_2^2 = \frac{1}{288} \sum_{i,j=1}^s \int_{G_s} \left(\frac{\partial^2 f}{\partial x^i \partial x^j} \right)^2 - \frac{1}{480} \sum_{i=1}^s \int_{G_s} \left(\frac{\partial^2 f}{\partial x^i \partial x^i} \right)^2.$$

Proof. From the (pairwise) independence of the x_r , we have

$$(9) \quad \sigma_{2N}^2(J_2) = \frac{1}{N^2} \sum_{r=1}^N \sigma^2 \left(\frac{f(x_r) + f(x'_r)}{2} \right).$$

Let

$$(10) \quad \tau_r = \sigma^2 \left(\frac{f(x_r) + f(x'_r)}{2} \right) = N \int_{A_r} \left(\frac{f(x) + f(x')}{2} - N \int_{A_r} \frac{f(x) + f(x')}{2} dx \right)^2 dx$$

where x' is, as before, the point of A_r symmetrically opposite x . For $x \in A_r$, we may under the assumptions of Theorem, write

$$(11) \quad \begin{aligned} f(x) &= f(c_r) + \sum_{i=1}^s (x^i - c_r^i) \frac{\partial f}{\partial x^i}(c_r) \\ &\quad + \frac{1}{2} \sum_{i,j=1}^s (x^i - c_r^i)(x^j - c_r^j) \frac{\partial^2 f}{\partial x^i \partial x^j}(c_r) + o(N^{-2/s}). \end{aligned}$$

For convenience I shall write “ f ” for $f(c_r)$, “ f_i ” for $\partial f(c_r)/\partial x^i$, “ f_{ij} ” for $\partial^2 f(c_r)/\partial x^i \partial x^j$ and “ δ^i ” for $x^i - c_r^i$. Then

$$(12) \quad \frac{f(x) + f(x')}{2} = f + \frac{1}{2} \sum_{i,j=1}^s \delta^i \delta^j f_{ij} + o(N^{-2/s}).$$

Now $N \int_{A_r} \delta^i \delta^j$ is zero if $i \neq j$, while

$$N \int_{A_r} (\delta^i)^2 = \frac{1}{12} N^{-2/s}.$$

Therefore

$$(13) \quad N \int_{A_r} \frac{f(x) + f(x')}{2} dx = f + \frac{N^{-2/s}}{24} \sum_{i=1}^s f_{ii} + o(N^{-2/s}).$$

From (10), (12), and (13) we get

$$(14) \quad \tau_r = N \int_{A_r} \left(\frac{1}{2} \sum_{i,j=1}^s \delta^i \delta^j f_{ij} - \frac{N^{-2/s}}{24} \sum_{i=1}^s f_{ii} + R \right)^2,$$

where $R = o(N^{-2/s})$.

Temporarily writing “ Σ ” for the total of the two sums in (14) we have

$$(15) \quad \tau_r = N \int_{A_r} \Sigma^2 + 2N \int_{A_r} R \Sigma + N \int_{A_r} R^2.$$

The last of these three terms is clearly $o(N^{-4/s})$; the same holds true for the second term, since $\delta^i = O(N^{-1/s})$ and so $\Sigma = O(N^{-2/s})$, and therefore

$$\left| N \int_{A_r} R \Sigma \right| \leq \left(N \int_{A_r} \Sigma^2 \right)^{1/2} \left(N \int_{A_r} R^2 \right) = O(N^{-2/s}) \cdot o(N^{-2/s}).$$

It follows that

$$(16) \quad \tau_r = N \int_{A_r} \left(\frac{1}{2} \sum_{i,j=1}^s \delta^i \delta^j f_{ij} - \frac{N^{-2/s}}{24} \sum_{i=1}^s f_{ij} \right)^2 + o(N^{-4/s}).$$

Calculating the integral in (16) is facilitated by noting that $\int_{A_r} \delta^i \delta^j \delta^k \delta^L$ is zero unless i, j, k, L are equal in pairs, and that

$$N \int_{A_r} (\delta^i)^2 (\delta^j)^2 = \frac{N^{-4/s}}{144} \text{ if } i \neq j, \quad N \int_{A_r} (\delta^i)^4 = \frac{N^{-4/s}}{80}.$$

We finally obtain:

$$(17) \quad \tau_r = \frac{N^{-4/s}}{288} \sum_{1 \leq i \neq j \leq s} f_{ij}^2 + \frac{N^{-4/s}}{720} \sum_{i=1}^s f_{ij}^2 + o(N^{-4/s}).$$

From (9), (10) and (17) we obtain

$$(18) \quad N^{1+4/s} \sigma_{2N}^2(J_2) = \frac{1}{288} \sum_{1 \leq i \neq j \leq s} \sum_{r=1}^N \frac{1}{N} \left(\frac{\partial^2 f}{\partial x^i \partial x^j} (c_r) \right)^2 + \frac{1}{720} \sum_{i=1}^s \sum_{r=1}^N \left(\frac{\partial^2 f}{\partial x^i \partial x^i} (c_r) \right)^2 + o(1).$$

Each inner sum in (18) is a Riemann sum, which approaches the integral (over G_s) of the function involved as $N \rightarrow \infty$.

Therefore

$$(19) \quad N^{1+4/s} \sigma_{2N}^2(J_2) = \frac{1}{288} \sum_{1 \leq i \neq j \leq s} \int_{G_s} \left(\frac{\partial^2 f}{\partial x^i \partial x^j} \right)^2 + \frac{1}{720} \sum_{i=1}^s \int_{G_s} \left(\frac{\partial^2 f}{\partial x^i \partial x^i} \right)^2 + o(1),$$

and the theorem follows.

We see then that for smooth functions J_2 converges to the integral somewhat faster than J_0 or J_1 . It is interesting to note, also, that J_2 is exact for linear integrands—so that the quantity d_2 is not a measure of the deviation of the integrand from constancy, as are d_0 and d_1 , but of its deviation from linearity.

For less smooth integrands J_2 may not be superior to J_1 ; but for a large class of functions which may even be discontinuous, both J_1 and J_2 are asymptotically better than J_0 , and in fact

$$(20) \quad \sigma_N(J_i) = O(N^{-(1/2+1/2s)}), \quad i = 1, 2.$$

To see this, let f be bounded in G_s , and piecewise smooth in the following sense: G_s may be broken up into a finite number of regions, with smooth boundaries, such that in the interior of each region all the second partial derivatives of f are continuous and bounded. Then for N large the number of subcubes A_r which do not lie wholly inside a single one of these regions will be $O(N^{1-1/s})$. For these subcubes τ_r will be bounded, since f is bounded on G_r ; for the remaining subcubes, $\tau_r = O(N^{-4/s})$ as in the proof of Theorem 1. Thus

$$\sigma_{2N}^2(J_2) = \frac{1}{N^2} \sum_{r=1}^N \tau_r \leq \frac{B_1 N^{1-s} + B_2 N(N^{-4/s})}{N^2}$$

and (20) follows for J_2 . In an exactly similar manner it follows for J_1 , under the weaker assumption that the first partial derivatives of f are continuous and bounded in each region, using the proof of Theorem 3 of MMC.

3. Related Methods. Two modifications of the proposed quadrature method were considered, that seem worth some comment. The first is simply a generalization, in which G_s is not necessarily partitioned into subcubes, but more generally into congruent subintervals in the manner described in the first paragraph of this paper. In MMC the estimate J_1 (there called J'') was treated in this more general manner, and it was seen that there might sometimes be a gain to partitioning the different coordinate axes differently. However, this does not seem to be the case for J_2 . If, in the general case, we impose the “regularity” condition of MMC on the partitions of G_s , and carry through the reasoning of the proof of the Theorem above, we obtain in place of (19):

$$(19') \quad N\sigma_{2N}^2(J_2) = \frac{1}{288} \sum_{1 \leq i \neq j \leq s} \frac{1}{n_i^2 n_j^2} \int_{G_s} \left(\frac{\partial^2 f}{\partial x^i \partial x^j} \right)^2 + \frac{1}{720} \sum_{i=1}^s \frac{1}{n_i^4} \int_{G_s} \left(\frac{\partial^2 f}{\partial x^i \partial x^i} \right)^2 + o(N^{-4/s}).$$

While, for given $N = n_1 \cdot n_2 \cdot \dots \cdot n_s$, the total of the 2 sums in (19') might be made smaller by choosing the n_i unequal than by choosing them equal, it is not likely that one would know in advance how to do this.

The second modification I considered was an attempt to halve the number of evaluations of the integrand needed for a given accuracy. For each A_r , instead of evaluating both $f(x_r)$ and $f(x_r')$, I proposed to choose at random a number α_r in between 0 and 1, set $x_r'' = \alpha x_r + (1 - \alpha)x_r'$, and calculate only $f(x_r'')$. However, the quantity

$$\frac{1}{N} \sum_{r=1}^N f(x_r'')$$

does not have mean value I in general, since x_r'' is not uniformly distributed on A_r . This can be compensated for by introducing a weight factor: For $x = (x^1, x^2, \dots, x^s)$ such that $-N^{-1/s} \leq x^i \leq N^{-1/s}$, let

$$(21) \quad \phi(x) = \left(2N^{1/s} \max_{1 \leq i \leq s} |x^i| \right)^{s-1}.$$

Then the estimator

$$J_4 = \frac{s-1}{N} \sum_{r=1}^N f(x_r'') \frac{\phi((2\alpha_r - 1)(x_r - c_r))}{1 - \phi((2\alpha_r - 1)(x_r - c_r))}$$

does have mean value I . However, it turns out to have infinite variance (though its expected absolute deviation from the mean is finite). In some numerical experiments on simple integrands, convergence to the integral was not apparent as N was raised up to 65,536; so the method seems worthless.

4. Automatic Error Estimation. One of the attractive features of simple Monte-Carlo is the ease with which the error of the quadrature may be estimated. Once $f(y_r)$ is calculated for each $1 \leq r \leq N$, a single arithmetic operation produces $f^2(y_r)$, so that $\int_{G_s} f^2$, and so d_0 and $\sigma_N(J_0)$, can be approximately evaluated in the course of the calculation of J_0 . In MMC I pointed out a method of evaluating $\sigma_N(J_1)$ by, in effect,

calculating two independent samples of J_1 . This method can be extended to J_2 . In each subcube A_r one chooses at random two points x_r and z_r , and finds x_r' and z_r' as above. The integral is then estimated by

$$(22) \quad J_2'(f, N) = \frac{1}{N} \sum_{r=1}^N \frac{f(x_r) + f(x_r') + f(z_r) + f(z_r')}{4}.$$

At the same time the quantity

$$(23) \quad D_2 = D_2(f, N) = \frac{1}{2N} \left(\sum_{r=1}^N \left(\frac{f(x_r) + f(x_r')}{2} - \frac{f(z_r) + f(z_r')}{2} \right)^2 \right)^{1/2}$$

is calculated; the expected value of D_2^2 is the variance of J_2' , so that D_2 can be taken as an estimate of the standard deviation of J_2' . The calculation of J_2' involves $4N$ evaluations of the integrand f , and

$$\sigma_{4N}(J_2') = \frac{1}{\sqrt{2}} \sigma_{2N}(J_2)$$

since J_2' is just the average of 2 independent samples of J_2 . This implies that using J_2' instead of J_2 involves a slight loss of accuracy, since by Theorem 1,

$$\sigma_{4N}(J_2) \approx \frac{1}{2^{1/2+2/s}} \sigma_{2N}(J_2)$$

if f is smooth. However, in my experience the importance of having a good estimate of the error is so great as to justify this loss of accuracy and the extra effort required to calculate D_2 .

Usually, in approximately evaluating an integral by the present methods, one would calculate $J_2(f, N)$ or $J_2'(f, N)$ for a few values of N , in ascending sequence. When J_2' is used, one could, for each value of N , also calculate $D_2 N^{1/2+2/s}$. If the asymptotic form of $\sigma_{2N}(J_2)$ given in the Theorem is, for the last two or three values of N used, a good approximation to the standard deviation, $D_2 N^{1/2+2/s}$ will be close to constant and its value (for the last value of N) may be taken as the value of $2^{-1/2} d_2$. Further calculations, with higher N , may thereafter be made using J_2 , and taking $d_2 N^{-(1/2+2/s)}$ as the standard deviation.

(For J_1 , automatic error estimation is achieved by using the estimator

$$J_1'(f, N) = \frac{1}{N} \sum_{r=1}^N \frac{f(x_r) + f(z_r)}{2}$$

to approximate I , and using

$$D_1(f, N) = \frac{1}{2N} \left(\sum_{r=1}^N (f(x_r) - f(z_r))^2 \right)^{1/2}$$

as the estimate of the standard deviation of J_1' . For convenience I shall also denote the above-mentioned estimate of the standard deviation of J_0 , i.e., the quantity

$$N^{-1/2} \left(\frac{1}{N} \sum_{r=1}^N f^2(y_r) - \left(\frac{1}{N} \sum_{r=1}^N f(y_r) \right)^2 \right)^{1/2}$$

by “ D_0 ”.)

TABLE I

| N | D_0 | D_1 | D_2 | $D_0N^{1/2}$ | $D_1N^{1/2+1/s}$ | $D_2N^{1/2+2/s}$ |
|--------|--------|---------|----------|--------------|------------------|------------------|
| 2^4 | .019 | .0085 | .0030 | .078 | .066 | .048 |
| 3^4 | .011 | .0037 | .00085 | .102 | .102 | .069 |
| 4^4 | .0064 | .0014 | .00028 | .102 | .092 | .073 |
| 5^4 | .0044 | .00085 | .00010 | .110 | .105 | .062 |
| 8^4 | .0018 | .00019 | .000016 | .115 | .098 | .068 |
| 10^4 | .0011 | .00010 | .0000068 | .113 | .099 | .068 |
| 16^4 | .00044 | .000024 | .0000011 | .112 | .100 | .069 |

TABLE I_a

| N | E_0 | E_1 | E_2 | r_0 | r_1 | r_2 |
|--------|---------|----------|------------|-------|-------|-------|
| 2^4 | -.00673 | -.00505 | .00159 | .35 | .59 | .53 |
| 3^4 | -.00401 | -.00557 | -.000039 | .36 | 1.50 | .05 |
| 4^4 | .000998 | .00080 | .000082 | .16 | .57 | .29 |
| 5^4 | .00256 | .00097 | -.000042 | .58 | 1.14 | .42 |
| 8^4 | -.00086 | .000065 | .0000088 | .48 | .34 | .55 |
| 10^4 | -.00124 | -.000090 | -.00000104 | 1.10 | .90 | .15 |
| 16^4 | -.00023 | .0000238 | .00000089 | .52 | .99 | .81 |

TABLE II

| N | D_0 | D_1 | D_2 | $D_0N^{1/2}$ | $D_1N^{1/2+1/s}$ | $D_2N^{1/2+2/s}$ |
|--------|-------|--------|---------|--------------|------------------|------------------|
| 2^4 | .17 | .11 | 0 | .68 | .91 | .00000 |
| 3^4 | .083 | .051 | .035 | .75 | 1.39 | 2.86 |
| 4^4 | .046 | .023 | .012 | .73 | 1.48 | 3.14 |
| 5^4 | .029 | .013 | .0056 | .72 | 1.58 | 3.49 |
| 8^4 | .011 | .0034 | .00098 | .71 | 1.74 | 4.00 |
| 10^4 | .0070 | .0018 | .00041 | .70 | 1.75 | 4.08 |
| 16^4 | .0028 | .00044 | .000064 | .71 | 1.80 | 4.17 |

TABLE II_a

| N | E_0 | E_1 | E_2 | r_0 | r_1 | r_2 |
|--------|-----------|---------|----------|-------|-------|-------|
| 2^4 | -.09922 | .1363 | 0 | .58 | 1.24 | |
| 3^4 | .07652 | .0481 | .02627 | .92 | .94 | .75 |
| 4^4 | -.05043 | .0372 | .00821 | 1.10 | 1.62 | .68 |
| 5^4 | -.01536 | .0261 | .000733 | .53 | 2.00 | .13 |
| 8^4 | -.00198 | .00243 | -.000158 | .18 | .71 | .16 |
| 10^4 | -.01132 | -.00092 | .000020 | 1.61 | .51 | .05 |
| 16^4 | -.0002285 | -.00066 | .0000412 | .08 | 1.50 | .64 |

5. Experiments. In order to test the accuracy of the error estimates above for smooth functions, and to see the behavior of J_1 and J_2 when the integrand is discontinuous, three 4-dimensional integrals were calculated. Tables I and I_a present the results for the calculation of

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 (\exp [x^1 \cdot x^2 \cdot x^3 \cdot x^4] - 1) dx^1 dx^2 dx^3 dx^4 = .0693976$$

and Tables II and II_a give the corresponding results for

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \sin 2\pi(x^1 + x^2 + x^3 + x^4) dx^1 dx^2 dx^3 dx^4 = 0 .$$

Here and below, $E_0, E_1,$ and E_2 are the actual errors of J_0, J_1' and J_2' respectively; and in each case $r_i = |E_i|/D_i$ —that is, the ratio of the actual error to the estimated standard deviation.

Table I shows that $D_0N^{1/2}, D_1N^{1/2+1/s},$ and $D_2N^{1/2+2/s}$ were substantially constant for $K \geq 3,$ indicating that the standard deviations were in close accordance with the predictions of the Theorem above and of Theorem 3 of MMC. The second integrand is more rapidly oscillating, with the result that in Table II $D_1N^{1/2+1/s}$ and $D_2N^{1/2+2/s}$ are approximately constant only for $K \geq 7.$ In both cases the D_i accurately estimate the standard deviations for moderate values of $N.$ The gain in accuracy due to J_2' is clear, though in comparing D_0 and D_1 to $D_2,$ D_0 should be divided by 2 and D_1 by 1.4 to compensate for the greater number of function evaluations done in the calculation of $J_2'.$

TABLE III

| N | D_0 | D_1 | D_2 | $D_0N^{1/2}$ | $D_1N^{1/2+1/2s}$ | $D_2N^{1/2+1/2s}$ |
|--------|-------|--------|--------|--------------|-------------------|-------------------|
| 2^4 | .108 | .076 | .044 | .43 | .43 | .25 |
| 3^4 | .051 | .032 | .017 | .46 | .49 | .26 |
| 4^4 | .029 | .015 | .0080 | .47 | .48 | .26 |
| 5^4 | .019 | .0079 | .0046 | .47 | .44 | .26 |
| 8^4 | .0073 | .0025 | .0014 | .46 | .46 | .24 |
| 10^4 | .0046 | .0014 | .00077 | .46 | .44 | .24 |
| 16^4 | .0018 | .00045 | .00023 | .46 | .46 | .24 |

TABLE III_a

| N | E_0 | E_1 | E_2 | r_0 | r_1 | r_2 |
|--------|---------|---------|---------|-------|-------|-------|
| 2^4 | .0584 | .0272 | -.0040 | .54 | .36 | .09 |
| 3^4 | -.0002 | .00060 | .00287 | 0 | .02 | .17 |
| 4^4 | -.0119 | -.00408 | -.00408 | .41 | .27 | .51 |
| 5^4 | -.0180 | -.00118 | -.00198 | .95 | .15 | .43 |
| 8^4 | -.0075 | -.00310 | -.00029 | 1.03 | 1.24 | .21 |
| 10^4 | -.00108 | .000275 | .00020 | .23 | .20 | .26 |
| 16^4 | -.00052 | .000114 | .000041 | .29 | .25 | .18 |

Tables III and III_a present the results of calculating the integral of the function given by

$$f(x^1, x^2, x^3, x^4) = 1 \text{ if } (x^1)^2 + (x^2)^2 + (x^3)^2 + (x^4)^2 \leq 1, \\ = 0 \text{ otherwise .}$$

This function is discontinuous in G_4 , and so in accordance with the discussion leading to (20), we should expect that D_1 and D_2 would go to zero as $N^{-(1/2+1/2s)}$. The approximate constancy of $D_1N^{1/2+1/2s}$ and $D_2N^{1/2+1/2s}$ in Table III confirms this very well for this simple integrand.

The values of r in Tables I_a, II_a, and III_a also conform to what is expected on the assumption that J_0 , J_1' and J_2' are approximately normally distributed. The r 's are mostly ≤ 1 , and are only rarely as high as 2. In practical calculations, of course, only the D_i are known and information about the actual errors is to be inferred from them; $2D_i$ is then a fairly safe ("5% confidence level") upper bound for $|E_i|$.

The following integral arose in a physical problem [3]:

$$(24) \quad \frac{10^4}{\pi^2 T^2} \int_0^{A(T)} \int_0^{\pi/2} k^2 \sin \theta \frac{2.07k^2 + .01 \sin^2 \theta}{we^{w/.0138T}} d\theta dk,$$

where

$$w = (4.285k^4 + .0414k^2 \sin^2 \theta)^{1/2};$$

it was to be evaluated to an accuracy of about 1 part in 100 for various values of the parameter T . As the region of integration is a rectangle, it was first attempted to do the calculation using the trapezoid rule in each dimension. In one dimension the trapezoid rule approximation converges as M^{-2} where M is the number of points used—if the integrand is sufficiently smooth. In two dimensions the approximations should then converge as M^{-1} . In this case however, they were found to converge only as $M^{-1/2}$. This is apparently due to the fact that the second derivative, with respect to k , of the integrand is infinite at the origin; and so it could not be corrected by substituting any higher-order quadrature rule for the trapezoid rule. The calculation was then done by the simple and modified Monte-Carlo methods under discussion, and the results (for $T = 10^{-5}$, $A(T) = 10^{-4}$) are given in Table IV.

TABLE IV

| N | J_0 | J_1' | J_2' | $D_0N^{1/2}$ | D_1N | $D_2N^{3/2}$ |
|------------------|-------|--------|--------|--------------|--------|--------------|
| 50 ² | .755 | .592 | .582 | 3.97 | 34.4 | 224 |
| 100 ² | .634 | .590 | .588 | 3.53 | 46.1 | 346 |
| 200 ² | .584 | .590 | .588 | 3.20 | 44.6 | 354 |
| 400 ² | .590 | .588 | .588 | 3.21 | 44.8 | 350 |

In this case the integrand satisfied the hypotheses of Theorem 3 of MMC, but not those of the theorem of the present paper. Thus the approximate constancy of $D_1N^{1/2+1/2s}$ was expected, but that of $D_2N^{1/2+2/2s}$ was surprising, and indicates a possibility of weakening the hypotheses of the theorem. Practically, the application of J_2' was successful: J_2' achieved the desired accuracy with $M = 10,000$, while with the trapezoid rule (improved by use of Richardson's "deferred approach to the limit"), it was necessary to go up to $M = 160,000$ and at that the results did not generate much confidence, as Richardson's extrapolation differed from the last trapezoidal value by about 7%.

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6. Comment. J_2' offers the advantage, over J_1' , of faster convergence to the integral. The improvement, for values of N for which the asymptotic error for a given level of effort and expressions are fairly accurate, is given by the factor $(\sqrt{2d_2/d_1}) N^{-1/8}$ by which the standard deviation is multiplied. This may in some cases be no improvement at all; d_2 might be sufficiently greater than d_1 to make this factor greater than 1 for all reasonable values of N . Now in calculating, J_2' , J_1' can be obtained simultaneously; and D_1 can also be gotten with very little extra effort. In doubtful situations, where it is not known how high an N will have to be used, it is advisable to do this for the first values of N tried, after which it can be seen whether J_1' or J_2' is the better estimator for the specific integral being studied.

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