

# A COMBINATION OF MONTE CARLO AND CLASSICAL METHODS FOR EVALUATING MULTIPLE INTEGRALS

BY SEYMOUR HABER

Communicated by E. Isaacson, February 29, 1968

1. **Stochastic quadrature formulas.** In the simplest "Monte Carlo" scheme for numerically approximating the integral

$$(1) \quad I = \int_{G_s} f(\mathbf{x}) d\mathbf{x}$$

( $G_s$  is the closed unit cube in  $E^s$ ),  $N$  points  $\mathbf{x}_1, \dots, \mathbf{x}_N$  are chosen at random in  $G_s$  and the quantity

$$J_0 = \frac{1}{N} \sum_{i=1}^N f(\mathbf{x}_i)$$

is taken as an estimate of  $I$ . The error analysis is probabilistic. Regarding the  $\mathbf{x}_i$  as (pairwise) independent random variables uniformly distributed on  $G_s$ ,  $J_0$  is a random variable with mean  $I$ ; the amount by which it is apt to differ from  $I$  is estimated in terms of its standard deviation  $\sigma(J_0)$ . In general (for  $f \in L^2(G_s)$ ),

$$\sigma(J_0) = C_0(f)N^{-1/2};$$

and it is usual to consider  $3\sigma$  (or even  $2\sigma$ ) as a reliable upper bound on  $|J - I|$ .

Let  $D_s^n$  denote the set of real functions  $f$  such that

$$\frac{\partial^{n_1 + \dots + n_s}}{(\partial x^1)^{n_1} \dots (\partial x^s)^{n_s}} f(x^1, x^2, \dots, x^s)$$

is continuous on  $G_s$  whenever  $n_1, n_2, \dots, n_s \leq n$ . N. S. Bahvalov [1], in a study of lower bounds on quadrature errors showed that for the class  $D_s^n$  the error of any nonrandom (e.g. Newton-Cotes, Gaussian) quadrature method is  $\Omega(N^{-n/s})$ ;<sup>1</sup> for random methods the best he could show was  $\sigma = \Omega(N^{-(n/s+1/2)})$  and he showed that for the set of periodic functions in  $D_s^n$  there in fact exist methods for which  $\sigma = O(N^{-(n/s+1/2)})$ .

In this note I shall give a general description of a class of formulas which combine the Monte Carlo and classical approaches to get

<sup>1</sup> Hardy's notation:  $f = \Omega(g)$  iff  $g = O(f)$ .

errors of the order of  $N^{-(n/s+1/2)}$  for the class  $D_s^n$ , and construct some specific formulas of this class for the case  $n=2$ . A more complete development, and proofs, will appear elsewhere.

DEFINITION. A "stochastic quadrature formula (s.q.f) of degree  $n$  (for  $G_s$ )" is a set of 1-dimensional random variables  $A_1, \dots, A_k$  and  $s$ -dimensional random variables  $\mathbf{X}_1, \dots, \mathbf{X}_k$ , such that

(1)  $\sum_{i=1}^k A_i P(\mathbf{X}_i) \equiv \int_{G_s} P$  whenever  $P$  is a polynomial (in  $s$  variables) of degree  $n$  or lower; but there is a polynomial  $P^*$  of degree  $n+1$  such that

$$\sum_{i=1}^k A_i P^*(\mathbf{X}_i) \neq \int_{G_s} P^*.$$

(2)  $m(\sum_{i=1}^k A_i f(\mathbf{X}_i)) = \int_{G_s} f$  whenever  $f \in L^2(G_s)$  (" $m(\cdot)$ " denotes the mean of a random variable).

For example,  $\mathbf{X}_1$  uniformly distributed over  $G_s$ ,  $\mathbf{X}_2 = (1/2, \dots, 1/2) - \mathbf{X}_1$ , and  $A_1 \equiv A_2 \equiv 1/2$  define an s.q.f. of degree 1.

I shall write " $Q(f)$ " for  $\sum_{i=1}^k A_i f(\mathbf{X}_i)$ , and speak of "the quadrature formula  $Q$ ." In the usual way one may apply  $Q$  to any region  $A$  obtainable from  $G_s$  by an affine transformation, without changing its degree. The adapted formula will be denoted by " $Q_{(A)}$ ." I shall denote by " $Q_M$ " the formula resulting from partitioning  $G_s$  into  $M$  congruent subcubes and applying  $Q$  to each. The number of function evaluations used in a quadrature formula will be denoted by " $N$ "; for  $Q_M$ ,  $N = kM$ .

THEOREM. If  $Q$  is a stochastic quadrature formula of degree  $n-1$  and  $f \in D_s^n$ , then

$$(2) \quad \sigma(Q_M(f)) \sim C(f)N^{-(n/s+1/2)}$$

where

$$(3) \quad C(f) = \frac{k^{n/s+1/2}}{2^{n+s}n!} \left( \sum_{i,j} m_{ij} \int_{G_s} f^{(i)} f^{(j)} \right)^{1/2}.$$

Here " $f(N) \sim g(N)$ " means  $f(N)/g(N) \rightarrow 1$  as  $N \rightarrow \infty$ . The sum in (3) runs over all  $n$ -tuples  $i$  and  $j$  of integers between 1 and  $s$ . The notations used are: If  $i = (i^1, i^2, \dots, i^n)$ ,  $j = (j^1, \dots, j^n)$ , then

$$f^{(i)} = \frac{\partial^n f}{(\partial x^{i^1}) \dots (\partial x^{i^n})}, \quad \mathbf{x}^{(i)} = x^{i^1} \cdot x^{i^2} \cdot \dots \cdot x^{i^n}$$

and

$$m_{ij} = m \left( \left( Q_{(A)}(\mathbf{x}^i) - \int_A \mathbf{x}^i \right) \left( Q_{(A)}(\mathbf{x}^j) - \int_A (\mathbf{x}^j) \right) \right)$$

where  $A = A_s$  is the cube  $|x^i| \leq 1, i = 1, 2, \dots, s$ .

$C(f)$  will rarely be known a priori; however a good a posteriori estimate of  $\sigma(Q_M(f))$  may be obtained by a modification of the calculation in the manner described in [3].

**2. Formulas of degree 2.** In [2] an s.q.f.  $Q$  of degree zero with  $k = 1$  was investigated; in [3] one of degree 1 with  $k = 2$  was given. For  $n \geq 2$  the situation is more complicated; it is a consequence of a theorem of Stroud [4], that

$$k \geq \binom{n + s}{[n/2]}$$

("[·]" denoting the greatest integer function), so that  $k$  cannot be independent of  $s$ . For constant coefficient formulas we have

**THEOREM.** *If*

$$Q(f) = \frac{1}{k} \sum_{i=1}^k f(\mathbf{X}_i)$$

*is an s.q.f. of degree  $\geq 2$  for  $G_s$ , then  $k \geq 3s + 1$ .*

**THEOREM.** *If  $(a_{i,j})$  is a  $(3s + 1) \times k$  real matrix such that*

- (1)  $a_{i,j} = k^{-1/2}$  for all  $j$ ,
  - (2)  $a_{i,1}^2 + a_{i,2}^2 + \dots + a_{i,k}^2 = 1$  for all  $i$ ,
  - (3)  $a_{i,1}a_{i',1} + a_{i,2}a_{i',2} + \dots + a_{i,k}a_{i',k} = 0$  if  $i \neq i'$ ,
  - (4)  $a_{i,j}^2 + a_{i+1,j}^2 + a_{i+2,j}^2 = 3/k$  for all  $j$  and for  $i = 2, 5, 8, \dots, 3s - 1$ ,
- we shall denote by " $V_L$ " ( $L = 1, 2, \dots, s$ ) the subspace of  $E^k$  spanned by the  $(3L - 1)$ st,  $3L$ th, and  $(3L + 1)$ st rows of  $(a_{i,j})$  and by " $S_L$ " the sphere of radius  $(3/k)^{1/2}$  in  $V_L$ , centered at the origin. Then if*

$$\mathbf{X}_j = (X_j^1, X_j^2, \dots, X_j^s), \quad j = 1, 2, \dots, k$$

*are random variables such that, for  $L = 1, 2, \dots, s$ ,*

$$(X_1^L, X_2^L, \dots, X_k^L)$$

*is uniformly distributed on  $S_L$ , then*

$$Q(f) = \frac{1}{k} \sum_{j=1}^k f(\mathbf{X}_j)$$

*is an s.q.f. of degree 2 for the cube  $A_s$ .*

It remains to be seen for which  $k$  such matrices exist; it is desirable that  $k$  be as low as possible. Here we have

THEOREM. *If there exists a Hadamard matrix ([5], [6]) of order  $r$ , then for any  $s$  such that  $3s+1 \leq r$ , there is a  $(3s+1) \times r$  matrix  $(a_{i,j})$  satisfying the conditions of the above theorem.*

For the top row of the Hadamard matrix  $H_r$  may be taken to have all entries = 1; and then the first  $3s+1$  rows of  $r^{-1/2}H_r$  satisfy all conditions.

Since Hadamard matrices of order  $r=4p$  are known to exist at least up to  $p=29$ ,  $k$  can be taken  $\leq 3s+4$  for  $s \leq 38$ ; and can in fact be taken equal to  $3s+1$  for  $s=1, 5, 9, \dots, 33$ .

The classical approaches to efficient quadrature have been: (1) To take advantage of as much smoothness as the integrand may have by constructing formulas of maximum degree using a fixed number of points; (2) To find formulas with a fixed number of points which minimize the error for functions with a given degree of smoothness. The second seems the more practical approach for functions of several variables, where smoothing is apt to be very difficult. With the present formulas, partitioning  $G_s$  reduces the error as quickly as possible for each fixed smoothness class  $D_s^n$ ; while the first approach continues in use, to reduce the number  $k$  in (3).

#### REFERENCES

1. N. S. Bahvalov, *On approximate calculation of multiple integrals*, Vestnik Moscow Univ. 4 (1959), 3-18.
2. S. Haber, *A modified Monte Carlo quadrature*, Math. Comp. 20 (1966), 361-368.
3. ———, *A modified Monte Carlo quadrature. II*. Math. Comp. 21 (1967), 388-397.
4. A. H. Stroud, *Quadrature methods for functions of more than one variable*, Ann. New York Acad. Sci. 86 (1960), 776-791.
5. J. Williamson, *Note on Hadamard's determinant theorem*, Bull. Amer. Math. Soc. 53 (1947), 608-613.
6. S. W. Golomb and L. D. Baumert, *The search for Hadamard matrices*, Amer. Math. Monthly 70 (1963), 12-17.

NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.