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

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

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

(G_s is the closed unit cube in E^s), N points $\mathbf{x}_1, \cdots, \mathbf{x}_N$ 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 3σ (or even 2σ) as a reliable upper bound on $|J-I|$.

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

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

is continuous on G_s whenever $n_1, n_2, \cdots, n_s \leqq n$. 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 $\Omega(N^{-n/s})$;[1] 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

[1] 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 $A_1, \cdots, A_k$ and s-dimensional random variables $X_1, \cdots, X_k$, such that

(1) $\sum_{i=1}^k A_iP(X_i) \equiv \int_{G_s} P$ 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

$$\sum_{i=1}^k A_iP^*(X_i) \not\equiv \int_{G_s} P^*.$$

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

For example, X_1 uniformly distributed over G_s, $X_2=(1/2, \cdots, 1/2)-X_1$, and $A_1 \equiv A_2 \equiv 1/2$ define an s.q.f. of degree 1.

I shall write "$Q(f)$" for $\sum_1^k A_if(X_i)$, 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*

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

where

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

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

$$f^{(i)} = \frac{\partial^n f}{(\partial x^{i_1})\cdot \cdots \cdot(\partial x^{i_n})}, \qquad \mathbf{x}^{(i)} = x^{i_1}\cdot x^{i_2}\cdot \cdots \cdot x^{i_n}$$

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 $|x^i| \leqq 1, i = 1, 2, \cdots, s$.

$C(f)$ 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 $n \geqq 2$ the situation is more complicated; it is a consequence of a theorem of Stroud [**4**], that

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

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

THEOREM. *If*

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

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

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) $a_{i,1}^2 + a_{i,2}^2 + \cdots + a_{i,k}^2 = 1$ *for all* i,

(3) $a_{i,1}a_{i',1} + a_{i,2}a_{i',2} + \cdots + a_{i,k}a_{i',k} = 0$ *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* $i = 2, 5, 8, \cdots, 3s-1$,

we shall denote by "V_L" $(L = 1, 2, \cdots, s)$ *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*

$$\boldsymbol{X}_j = (\overset{1}{X}_j, \overset{2}{X}_j, \cdots, \overset{s}{X}_j), \qquad j = 1, 2, \cdots, k$$

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

$$(\overset{L}{X}_1, \overset{L}{X}_2, \cdots, \overset{L}{X}_k)$$

is uniformly distributed on S_L, *then*

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

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* $3s+1 \leqq r$, *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 $\leqq 3s+4$ for $s \leqq 38$; and can in fact be taken equal to $3s+1$ for $s=1, 5, 9, \cdots, 33$.

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).

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