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

\[ I = \int_{G} f(x) \, dx \]

\((G, \text{ is the closed unit cube in } E^d), N \text{ points } x_1, \ldots, x_N \text{ are chosen at random in } G, \text{ and the quantity}

\[ J_0 = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \]

is taken as an estimate of \( I \). The error analysis is probabilistic. Regarding the \( x_i \) as (pairwise) independent random variables uniformly distributed on \( G, J_0 \) 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 \( f \in L^1(G) \)),

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

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

Let \( D^n \) denote the set of real functions \( f \) such that

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

is continuous on \( G \) whenever \( n_1, n_2, \ldots, n_s \leq n \). N. S. Bahvalov [1], in a study of lower bounds on quadrature errors showed that for the class \( D^n \) the error of any nonrandom (e.g. Newton-Cotes, Gaussian) quadrature method is \( \Omega(N^{-n/s}) \); 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 \( D^n \) 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

\[ \sigma = \Omega(g) \iff g = O(f). \]

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errors of the order of \( N^{-(n/2+1/2)} \) for the class \( D^n \), 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 \( A_1, \ldots, A_k \) and \( s \)-dimensional random variables \( X_1, \ldots, X_k \), such that

1. \( \sum_{i=1}^k A_i P(X_i) = \int_{G_s} P \) 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

\[
\sum_{i=1}^k A_i P^*(X_i) \neq \int_{G_s} P^*.
\]

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 \( G_1 \), \( X_2 = (1/2, \ldots, 1/2) - X_1 \), and \( A_1 = A_2 = 1/2 \) define an s.q.f. of degree 1.

I shall write \( \sigma_Q(f) \) for \( \int A_i f(X_i) \), 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 \( f \in D^n \), then

\[
\sigma(Q_M(f)) \sim C(f) N^{-(n/2+1/2)}
\]

where

\[
C(f) = \left( 2^{n+s} n! \right)^{1/2} \left( \sum m_{ij} \int_{G_s} f(x_i)f(x_j) \right)^{1/2}.
\]

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 \( i = (i^1, i^2, \ldots, i^n), j = (j^1, \ldots, j^n) \), then

\[
f^{(i)} = \frac{\partial^n f}{\partial x^{i_1} \cdots \partial x^{i_n}}, \quad x^{(i)} = x^{i_1}x^{i_2} \cdots x^{i_n}
\]

and

\[
m_{ij} = m \left( \left( Q_A(x^i) - \int_A x^i \right) \left( Q_A(x^j) - \int_A x^j \right) \right)
\]
where \( A = A_s \) is the cube \( |x^i| \leq 1, i = 1, 2, \ldots, s \).

\( C(f) \) 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

\[
 k \geq \left\lceil \frac{n + s}{n/2} \right\rceil
\]

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

**Theorem.** If

\[
 Q(f) = \frac{1}{k} \sum_{i=1}^{k} f(X_i)
\]

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. \( a_{i,1}^2 + a_{i,2}^2 + \cdots + a_{i,k}^2 = 1 \) 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. \( a_{i,j}^2 + a_{i+1,j}^2 + a_{i+s,j}^2 = 3/k \) for all \( j \) and for \( i = 2, 5, 8, \ldots, 3s - 1 \),

we shall denote by \( V_L \) \((L = 1, 2, \ldots, s)\) the subspace of \( \mathbb{R}^n \) spanned by the \((3L - 1)st, 3Lth, \) 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

\[
 X_j = (X_{j,1}, X_{j,2}, \ldots, X_{j,k}) \quad j = 1, 2, \ldots, k
\]

are random variables such that, for \( L = 1, 2, \ldots, s \),

\[
 (X_1^L, X_2^L, \ldots, X_k^L)
\]

is uniformly distributed on \( S_L \), then

\[
 Q(f) = \frac{1}{k} \sum_{i=1}^{k} f(X_i)
\]

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 \([S], [6]\) 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 \(s = 1, 5, 9, \ldots, 33\).

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 \(D_s\); while the first approach continues in use, to reduce the number \(k\) in (3).

**REFERENCES**


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