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PROCEDURES FOR MULTIPLE INTEGRATION

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Abstract—This paper presents a brief description of a numerical procedure for evaluating multiple integrals over the unit cube in N-dimensional space, for $N = 2, \ldots, 8$. A familiar smoothing process enhances the speed and accuracy. Examples are given.

We consider integrals over the unit cube $C : 0 \le x_i \le 1$ $(i = 1, \ldots, N)$ in N-dimensional space. We start with the well-established formula [1, pp. 142–163]:

$$\int \cdot_{C}\cdot \int f(x_1, \ldots, x_N)\, dx_1 \ldots dx_N \approx \left(\frac{1}{p}\right) \sum_{k=1}^{p} f\left(\left\{\frac{k\, c_1}{p}\right\}, \ldots, \left\{\frac{k\, c_N}{p}\right\}\right), \tag{1}$$

where $\{x\}$ is the fractional part of x. To improve results, we make the well-known polynomial substitutions [2, pp. 124–130]:

$$x_i = P_\alpha(x_i'), \qquad i = 1, \ldots, N, \tag{2}$$

where P_α is of degree α, before applying (1). Here, P_α is monotone and $P_\alpha(0) = 0$, $P_\alpha(1) = 1$.

The principal novelties are the following: (i) the integer vector $c = (c_1, \ldots, c_N)$ and the integer $p > 1$ are chosen, after a long and elaborate search and test procedure, to give good accuracy; (ii) a correction is made for a flaw in the usual naive application of the substitution (2).

Choices of c and p

In general, we use a c of the form $(1, s, \mathrm{mod}(s^2, p), \ldots \mathrm{mod}(s^{N-1}, p))$, where $\mathrm{mod}(b, p)$ is the integer between 0 and $p - 1$, inclusive, congruent to $b \bmod p$. For example, for $N = 3$, as one choice, we use $p = 2331$ and $s = 988$, so that $c = (1, 988, 1786)$.

For each $N = 2, 3, \ldots, 8$, ten good choices of p and s have been found. For each N, these choices $(p_1, s_1), \ldots, (p_{10}, s_{10})$ have $1 < s_i < p_i$ and $p_1 < p_2 < \cdots < p_{10}$; typically, they give a sequence of ten approximations which appear to close in on a value for the integral. Thus, for $f = [(1 + x_1^2)(1 + x_2^2)(1 + x_3^2)]^{-1}$ and $\alpha = 5$, one obtains the sequence .4882 7250, .4844 3705, .4844 7522, ... 7476, ... 7304, ... 7308, ... 7308, ... 7308 (only the last 4 decimals places are shown after the third approximation, since the first 4 repeat). The exact value is 0.48447307 (to 8 places).

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Correction of the Flaw in Polynomial Substitution

A good numerical integration procedure should integrate constant functions exactly. The use of the substitution (2) followed by application of (1) fails to meet this requirement. For it is equivalent to computing a "weighted" average of the values of f at p points of C. But the sum of the "weights" is, in general, not equal to 1. Thus, an error occurs for $f \equiv$ const. To eliminate it, one need only multiply the sum in (1) by the appropriate factor.

A similar flaw arises if one evaluates an iterated integral, such as

$$\int_a^b \int_{\Phi(x)}^{\theta(x)} f(x,y)\,dy\,dx,$$

by the familiar method of writing it as

$$\int_a^b g(x)\,dx,$$

and integrating this using a weighted average of values of g at $x_1, \dots, x_N$, then evaluating each $g(x_i)$ using a weighted average of values of $f(x_i, y)$ at $y_{i1}, \dots, y_{iN}$. The resulting approximation of the integral is, in general, not exact for $f \equiv 1$.

Further Examples

(a) $f = \exp(-x_1 x_2 x_3 x_4)$. Exact value: 0.9430 8257. Approximations: 0.9422 3615, 0.9429 6988, 0.9430 6899, ... 8394, ... 8128, ... 7706, ... 7840, ... 8238, ... 8237, ... 8266.
(b) $f = \sin(10 x_1 x_2 x_3 x_4 x_5 x_6)$. Exact value: 0.1279 4385. Approximations: 0.1339 1372, 0.1270 8588, 0.1274 7138, 0.1285 1864, 0.1280 5595, ... 3985, ... 0822, 0.1279 4979, ... 4640, ... 4264.
(c) $f = (x_1 x_2 \cdots x_8)^{-1/2}$(improper integral). Exact value: 256. Approximations: 159.10821, 190.37757, 253.65332, 255.83547, 255.83030, 255.47852, 255.46981, 256.61489, 256.06273, 256.01225.

Software has been written in FORTRAN 77 that computes the successive approximations as far as desired, up to the tenth, with a choice of 5 polynomials P_α of successively higher degree. The above examples use $P_5(t) = 10t^3 - 15t^4 + 6t^5$. A hardware implementation in the form of a dedicated integrated circuit (chip) has also been designed.

Computing times on an IBM 3090 computer, for examples such as those given above, vary from about 0.001 seconds for $N = 2$ in the first approximation, to about 4.5 seconds for $N = 8$ in the tenth approximation. The times are roughly proportional to the number p of function evaluations, and p varies from numbers less than 100 to numbers close to 50,000.

Tests have also been run on IBM-compatible PCs of several configurations. On a moderately capable PC (80286 processor running at 10 MHz with an 80287 math co-processor), the computing times required should be around 50 times larger than those mentioned above. With state-of-the-art hardware, e.g., 80486 @ 30–50 MHz, these times could be reduced quite substantially.

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