Error Bounds in Gaussian Integration of Functions of Low-Order Continuity

By Philip Rabinowitz

The standard error term in the Gaussian integration rule with N points involves the derivative of order $2N$ of the integrand. This seems to indicate that such a rule is not efficient for integrating functions of low-order continuity, i.e. functions which have only a few derivatives in the entire interval of integration. However, Stroud and Secrest [3] have shown that Gaussian integration is efficient even in these cases. By applying Peano's theorem [1, p. 109] to functions of low-order continuity, they have tabulated error coefficients $e_{m,N}$ by which the error in integrating such functions can be bounded, provided that a bound M_m exists for the derivative of order m of the integrand. In this case,

$$|E_N(f)| = \left| \int_{-1}^{1} f(x)dx - \sum_{i=1}^{N} w_i f(x_i) \right| \leqq e_{m,N} M_m \tag{1}$$

where $|f^{(m)}(x)| \leqq M_m$ in $I = \{-1 \leqq x \leqq 1\}$. In the present paper, we use results from the theory of Chebyshev expansions to compute a different set of error coefficients $d_{m,N}$ which provide sharper bounds on $E_N(f)$ in some cases.

Let $f(x)$ be continuous and of bounded variation in I. Then there is an expansion of the form

$$f(x) = \tfrac{1}{2}a_0 + a_1 T_1(x) + a_2 T_2(x) + \cdots = \sum_{n=0}^{\infty}{}' a_n T_n(x) \tag{2}$$

which is uniformly convergent throughout I. Here, $T_n(x)$ are the Chebyshev polynomials of the first kind and

$$a_n = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_n(x)}{(1-x^2)^{1/2}} dx = \frac{2}{\pi} \int_0^{\pi} g(\theta) \cos n\theta d\theta \tag{3}$$

where $g(\theta) \equiv f(\cos \theta)$. By integrating the right-hand integral in (3) successively by parts and applying the second mean-value theorem of the integral calculus after each integration, we get the following results of interest to us. These results as well as additional ones appear in Elliott [2].

A. Define $F_1(x) \equiv (1 - x^2)^{1/2} f'(x)$; if $F_1(x)$ is of bounded variation in I with $|F_1(x)| \leqq P_1$ and if C_1 is the number of intervals in I, in each of which $F_1(x)$ is monotonic, then

$$|a_n| \leqq 4C_1 P_1 / \pi n^2 \quad \text{for} \quad n \geqq 1\,. \tag{4}$$

B. Define $F_2(x) \equiv (1 - x^2) f''(x) - x f'(x)$; if $F_2(x)$ is of bounded variation in I with $|F_2(x)| \leqq P_2$, if C_2 is the number of intervals in I, in each of which $F_2(x)$ is monotonic, and if $\lim_{x \to \pm 1} F_1(x) = 0$, then

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(5) $$|a_n| \leqq 4C_2P_2/\pi n^3 \quad \text{for} \quad n \geqq 1\,.$$

Let us now apply the operator E_N to (2). We get

(6) $$E_N(f) = E_N\left(\sum_{n=0}^{\infty}{}' a_nT_n(x)\right) = \sum_{n=0}^{\infty}{}' a_nE_N(T_n) = \sum_{n=2N}^{\infty} a_nE_N(T_n)$$

since $E_N(T_n) = 0$ for $n < 2N$. If now $f(x)$ satisfies the conditions A, we get

(7) $$|E_N(f)| \leqq \frac{4C_1P_1}{\pi}\sum_{n=2N}^{\infty}\frac{|E_N(T_n)|}{n^2} = d_{1,N}C_1P_1$$

where

(8) $$d_{1,N} = \frac{4}{\pi}\sum_{n=2N}^{\infty}\frac{|E_N(T_n)|}{n^2}$$

converges since $|E_N(T_n)| \leqq 2 + 2/(n^2 - 1)$. This bound holds since $|T_n(x)| \leqq 1$ in I and $\sum_{i=1}^{N} w_i = 2$ implying that $|\sum_{i=1}^{N} w_iT_n(x_i)| \leqq 2$ and since $\int_{-1}^{1} T_n(x)dx = 2/(n^2 - 1)$. If $f(x)$ satisfies conditions B, we get similarly

(9) $$|E_N(f)| \leqq d_{2,N}C_2P_2$$

where

(10) $$d_{2,N} = \frac{4}{\pi}\sum_{n=2N}^{\infty}\frac{|E_N(T_n)|}{n^3}\,.$$

In Table 1, values of $e_{i,N}$ and $d_{i,N}$ are given for $i = 1, 2$ and $N = 4(3)16$. We see that $d_{i,N}/e_{i,N} < 1$ and that this ratio decreases with increasing N. Hence, in cases where C_iP_i is not too much greater than M_i, (7) and (9) will provide sharper error bounds than (1), especially for large N.

TABLE 1

N	$e_{1,N}$	$d_{1,N}$	$e_{2,N}$	$d_{2,N}$
4	2.76(−1)	8.64(−2)	2.19(−2)	7.07(−3)
7	1.65(−1)	3.13(−2)	7.63(−3)	1.50(−3)
10	1.18(−1)	1.60(−2)	3.86(−3)	5.40(−4)
13	9.15(−2)	9.68(−3)	2.33(−3)	2.54(−4)
16	7.48(−2)	6.48(−3)	1.56(−3)	1.39(−4)

Examples. 1. $f(x) = |x|^{4/3}$. In this case, $f''(x)$ is unbounded in I so that using (1), we find $E_N(f) \leqq e_{1,N}M_1$. Taking $N = 16$ and $M_1 = 4/3$, we find $E_{16}(f) \leqq 1.0(-1)$. Using (7) with $C_1 = 3$ and $P_1 = .92$, we find $E_{16}(f) \leqq 1.8(-2)$. The actual error is $1.0(-3)$. For $N = 4$, the figures are $3.7(-1)$, $2.4(-1)$, and $2.2(-2)$, respectively.

2. $f(x) = |x|^{8/3}$. In this case, $E_N(f) \leqq e_{2,N}M_2$. With $N = 16$ and $M_2 = 40/9$, we find $E_{16}(f) \leqq 7.0(-3)$. Using (9) with $C_2 = 3$ and $P_2 = 8/3$, we find $E_{16}(f) \leqq 1.2(-3)$. The actual error is $3.5(-5)$. For $N = 4$, the figures are $9.8(-2)$, $5.7(-2)$ and $5.1(-3)$, respectively.

3. $f(x) = (x + 1)^{5/4}$. In this case also, $f''(x)$ is unbounded in I so that $E_N(f) \leqq e_{1,N}M_1$. With $N = 16$ and $M_1 = (5/4)2^{1/4}$ we find $E_{16}(f) \leqq 1.1(-1)$. However, $F_2(x)$ satisfies conditions B so that we can use (9). With $C_2 = 2$ and $P_2 = (5/4)2^{1/4}$, we find $E_{16}(f) \leqq 4.2(-4)$. The actual error is $8.9(-7)$.

Remarks. 1. This method is not restricted to Gaussian rules but is applicable to any integration rule defined over I which integrates constants exactly. This includes the Lobatto, Radau, Newton-Cotes, Romberg and Gauss-Jacobi rules.

2. This method can be extended to cases where higher derivatives exist. Thus, Elliott [2] gives the estimate $|a_n| \leqq 4C_3P_3/\pi n^4$ where

$$F_3(x) \equiv (1 - x^2)^{1/2}[(1 - x^2)f'''(x) - 3xf''(x) - f'(x)]$$

satisfies conditions similar to B. However, the expressions for F_i become very complicated with increasing i and it is not worth the effort to find C_i and P_i.

3. Elliott also gives the estimate $|a_n| \leqq 4C_0P_0/\pi n$ where $F_0(x) \equiv f(x)$. However, it is probably not possible to use this method for functions with unbounded first derivatives. This is so since $\sum_{n=2N}^{\infty} |E_N(T_n)|/n$ probably diverges. This assumption is based on the fact that for Gauss-Chebyshev integration, we can prove divergence. The Gauss-Chebyshev integration rule is of the form

$$\int_{-1}^{1} \frac{f(x)}{(1 - x^2)^{1/2}}\, dx = \frac{\pi}{N} \sum_{i=1}^{N} f(x_i) + E_N(f) \tag{11}$$

where

$$x_i = \cos \frac{2i - 1}{2N}\pi, \qquad i = 1, \cdots, N. \tag{12}$$

Since $\int_{-1}^{1} T_n(x)/(1 - x^2)^{1/2}dx = 0$ for $n \geqq 1$, it follows that $E_N(T_n) = (\pi/N) \sum_{i=1}^{N} T_n(x_i)$. Since $T_n(x) = \cos (n \arccos x)$, we have $T_n(x_i) = \cos ((2i - 1)n\pi/2N)$. Hence, for $n = 2KN$, $K = 1, 2, \cdots$, $E_N(T_n) = -\pi$, from which it follows that $\sum_{n=2N}^{\infty} |E_N(T_n)|/n$ diverges.

Conclusions. As Examples 1 and 2 indicate, error bounds (1), (7) and (9) may give rather good bounds on the integration error. On the other hand, Example 3 shows that the bounds may overshoot the actual error by many orders of magnitude. Nevertheless, in the absence of further information, they are the best available for functions of low-order continuity. Since $|F_1(x)| \leqq |f'(x)|$ in I, (7) will be better than (1) for small values of C_1. The situation with F_2 is more complicated but usually P_2 will be of the same order of magnitude as M_2 so that (9) will give a better bound than (1) for small values of C_2. In both cases, the critical value of C_i increases with N. In cases when the singularity is at an endpoint of I, our method may be very advantageous. As Example 3 shows, we can use (9) even when $f''(x)$ is unbounded. More generally, $f^{(j)}(x)$ may be unbounded while $F_{j+k}(x)$ is well behaved, $k = 0, 1, \cdots$. But as mentioned above, the work involved in calculating C_{j+k} and P_{j+k} becomes prohibitive. On the other hand, (1) has the advantage of simplicity especially when compared with (9), and, of course, (1) is preferable when C_i is large. Hence there is room for both types of error bound.

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An Explicit Sixth-Order Runge-Kutta Formula

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1. Introduction. The system of ordinary differential equations considered has the form

$$dy/dx = f(x, y)\,, \qquad y(x_0) = y_0\,. \tag{1}$$

Here $y(x)$ and $f(x, y)$ are vector-valued functions

$$y(x) = (y_1(x), y_2(x), \cdots, y_m(x))\,,$$
$$f(x, y) = (f_1(x, y), f_2(x, y), \cdots, f_m(x, y))\,,$$

so that we are dealing with m simultaneous first-order equations.

For the fifth-order case, explicit Runge-Kutta formulas have been found whose remainder, while of order six when y is present in (1), does become of order seven when f is a function of x alone [3], [4]. This is due to the use of six functional substitutions, a necessary feature when y occurs nontrivially [1].

A family of explicit sixth-order formulas has been described [1]. In this family is the formula given in the next section. Its remainder, while of order seven when y is present in (1), is of order eight when f is a function of x alone. Here again the possibility arises because seven functional substitutions are used, rather than six. Once more, this is a necessity [2].

For selected equations (those not strongly dependent on y) such formulas seem to lead to some increase in accuracy.

2. Presentation of the Formula. For the interval $[x_n, x_n + h]$, Lobatto quadrature points leading to a remainder of order eight are

$$x_n, \qquad x_n + h/2, \qquad x_n + (7 - (21)^{1/2})h/14, \qquad x_n + (7 + (21)^{1/2})h/14, \qquad x_n + h.$$

A set of Runge-Kutta formulas related thereto is given below. They can be verified by substitution in the relations given by Butcher [1].

Expressed in a usual form they are

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