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,

\[
|E_N(f)| = \left| \int_{-1}^{1} f(x) dx - \sum_{i=1}^{N} w_if(x_i) \right| \leq e_{m,N}M_m
\]

where \( |f^{(m)}(x)| \leq M_m \) in \( I = [-1, 1] \). 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

\[
f(x) = \frac{1}{2}a_0 + a_1T_1(x) + a_2T_2(x) + \cdots + \sum_{n=0}^{\infty} a_nT_n(x)
\]

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

\[
a_n = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x)T_n(x)}{(1 - x^2)^{1/2}} dx = \frac{2}{\pi} \int_{0}^{\pi} g(\theta) \cos n\theta d\theta
\]

where \( g(\theta) = f(\cos \theta) \). 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 \( F_1(x) = (1 - x^2)^{1/2}f'(x) \); if \( F_1(x) \) is of bounded variation in \( I \) with \( |F_1(x)| \leq P_1 \) and if \( C_1 \) is the number of intervals in \( I \), in each of which \( F_1(x) \) is monotonic, then

\[
|a_n| \leq 4C_1P_1/\pi n^2 \quad \text{for} \quad n \geq 1.
\]

B. Define \( F_2(x) = (1 - x^2)f''(x) - xf'(x) \); if \( F_2(x) \) is of bounded variation in \( I \) with \( |F_2(x)| \leq P_2 \), 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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Let us now apply the operator $E_N$ to (2). We get

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

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

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

where

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

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

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

where

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

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

<table>
<thead>
<tr>
<th>$N$</th>
<th>$e_{1,N}$</th>
<th>$d_{1,N}$</th>
<th>$e_{2,N}$</th>
<th>$d_{2,N}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2.76(-1)</td>
<td>8.64(-2)</td>
<td>2.19(-2)</td>
<td>7.07(-3)</td>
</tr>
<tr>
<td>7</td>
<td>1.65(-1)</td>
<td>3.13(-2)</td>
<td>7.63(-3)</td>
<td>1.50(-3)</td>
</tr>
<tr>
<td>10</td>
<td>1.18(-1)</td>
<td>1.60(-2)</td>
<td>3.86(-3)</td>
<td>5.40(-4)</td>
</tr>
<tr>
<td>13</td>
<td>9.15(-2)</td>
<td>9.68(-3)</td>
<td>2.33(-3)</td>
<td>2.54(-4)</td>
</tr>
<tr>
<td>16</td>
<td>7.48(-2)</td>
<td>6.48(-3)</td>
<td>1.56(-3)</td>
<td>1.39(-4)</td>
</tr>
</tbody>
</table>

Examples. 1. $f(x) = |x|^{13}$. In this case, $f''(x)$ is unbounded in $I$ so that using (1), we find $E_N(f) \leq e_{1,N}M_1$. Taking $N = 16$ and $M_1 = 4/3$, we find $E_{16}(f) \leq 1.0(-1)$. Using (7) with $C_1 = 3$ and $P_1 = .92$, we find $E_{16}(f) \leq 1.8(-2)$. 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. $f(x) = |x|^{5/8}$. In this case, $E_N(f) \leq e_{2,N}M_2$. With $N = 16$ and $M_2 = 40/9$, we find $E_{16}(f) \leq 7.0(-3)$. Using (9) with $C_2 = 3$ and $P_2 = 8/3$, we find $E_{16}(f) \leq 1.2(-3)$. 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. \( f(x) = (x + 1)^5 \). In this case also, \( f''(x) \) is unbounded in \( I \) so that \( E_N(f) \leq e_{1,N}M_1 \). With \( N = 16 \) and \( M_1 = (5/4)2^{1/4} \) we find \( E_{16}(f) \leq 1.1(-4) \). 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 \( E_{16}(f) \leq 4.2(-4) \). 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 \( |a_n| \leq 4C_3P_3/\pi n^4 \) where

\[
F_3(x) = (1 - x^2)^{1/2}[(1 - x^2)f'''(x) - 3xf''(x) - f'(x)]
\]
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 \( |a_n| \leq 4C_3P_3/\pi n^4 \) 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

\[
\int_{-1}^{1} \frac{f(x)}{(1 - x^2)^{1/2}} dx = \frac{\pi}{N} \sum_{i=1}^{N} f(x_i) + E_N(f)
\]

where

\[
x_i = \cos \frac{\pi(i - 1)}{2N} \pi, \quad i = 1, \ldots, N.
\]

Since \( \int_{-1}^{1} T_n(x)/(1 - x^2)^{1/2} dx = 0 \) for \( n \geq 1 \), 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 \( n = 2KN, \quad K = 1, 2, \ldots, E_N(T_n) = -\pi \), 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 \( |F_1(x)| \leq |f''(x)| \) 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, \( k = 0, 1, \ldots \). 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.
An Explicit Sixth-Order Runge-Kutta Formula

By H. A. Luther

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

\[ \frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0. \]

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

\[ x_n, \quad x_n + h/2, \quad x_n + (7 - (21)^{1/2})h/14, \quad x_n + (7 + (21)^{1/2})h/14, \quad x_n + h. \]

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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