MATHEMATICS OF COMPUTATION, VOLUME 26, NUMBER 119, JULY, 1972

Numerical Quadrature by the ϵ-Algorithm

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Abstract. Modifications of Romberg's integration method are applicable to functions with endpoint singularities. Several authors have reached different conclusions on the usefulness of these schemes due to the potential difficulties in calculating certain exponents in the asymptotic error expansion. In this paper, we consider a method based on the ϵ-algorithm which does not require the user to supply these parameters. Tests show this luxury produces a method substantially better than the unmodified Romberg's method, but not as good as the modified procedure which assumes all the exponents are known. It is possible to design a scheme which incorporates the best of both methods and allows the user to decide how much information he wishes to provide. The algorithm is stable numerically in quadrature applications and converges for functions with endpoint singularities of an algebraic or logarithmic nature.

1. Introduction and Summary. Let $If = \int_0^1 f(x)\,dx$, and let a trapezoidal rule estimate of If be

$$Q_h f = h\left\{\frac{f(0)}{2} + \sum_{k=1}^{m-1} f(kh) + \frac{f(1)}{2}\right\}, \qquad h = \frac{1}{m}. \tag{1}$$

When $m = 2^n$, $n = 0, 1, 2, \cdots$, consider the sequence of such estimates

$$T_0^{(n)} \equiv Q_h f, \qquad h = 1/2^n, \qquad n = 0, 1, \cdots . \tag{2}$$

In this paper, we examine four extrapolation procedures (defined in Section 2) utilizing this data: (a) classical unmodified Romberg quadrature, (b) modified Romberg quadrature, (c) Aitken's del-square process, and (d) the ϵ-algorithm. Our results strongly indicate that in the case when f has an integrable endpoint singularity of algebraic or logarithmic nature, (d) is a viable alternative to (a), (b), and (c), since (a) and (c) may converge quite slowly and (b) may be inconvenient to implement.

2. Four Extrapolation Procedures. Let $(I - Q_h)f = E(h, f)$.
If $f \in C^{(2k+1)}[0, 1]$,

$$E(h, f) \sim a_1 h^2 + a_2 h^4 + \cdots + a_k h^{2k} + O(h^{2k+1}), \qquad h \to 0, \tag{3}$$

Received July 27, 1971, revised November 29, 1971.

AMS 1970 *subject classifications.* Primary 65B05, 65D30.

Key words and phrases. ϵ-algorithm, acceleration of convergence, extrapolation, numerical quadrature.

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where

$$a_j = (-1)^j \frac{|B_{2j}|}{(2j)!} (f^{(2j-1)}(1) - f^{(2k-1)}(0)), \tag{4}$$

(B_{2j} is the $2j$th Bernoulli number). If f has period 1 and is of class $C^{2k+1}[-\infty, \infty]$, all the a_j's are zero and $E(h, f) = O(h^{2k+1})$ [1]. In this case, none of the procedures described below will be appropriate.

Classical unmodified Romberg quadrature [1], [2] computes $T_0^{(0)}, T_0^{(1)}, \cdots$ and then combines them linearly to eliminate successive terms in the error expansion $E(h, f)$, i.e., computes $T_0^{(r+1)}$ from (1) and then $T_1^{(r)}, T_2^{(r-1)}, \cdots, T_{r+1}^{(0)}$ in turn, according to

$$T_k^{(m)} = (4^k T_{k-1}^{(m+1)} - T_{k-1}^{(m)})/(4^k - 1). \tag{5}$$

Unless $a_1 = a_2 = \cdots = a_{k-1} = 0$, the sequence $\{T_k^{(0)}\}$ converges to If faster than $\{T_0^{(k)}\}$.

Recently, generalizations of the Euler-Maclaurin formula, on which (3) and (4) are based, have appeared [3], [4], [5], [6], and [7]. In the case when $f(x)$ has an integrable algebraic singularity at an endpoint, (3) is replaced by

$$E(h, f) \sim b_1 h^{\alpha_1} + b_2 h^{\alpha_2} + \cdots + b_k h^{\alpha_k} + O(h^{\alpha_{k+1}}), \quad 0 < \alpha_1 < \alpha_2 < \cdots. \tag{6}$$

For example, if $f(x) = \sqrt{x} g(x)$ with $g(x)$ sufficiently differentiable and $g(0) \neq 0$,

$$E(h, f) \sim b_1 h^{3/2} + b_2 h^2 + b_3 h^{5/2} + b_4 h^{7/2} + o(h^{7/2}), \qquad h \to 0.$$

If one uses unmodified Romberg quadrature (5) on $\sqrt{x} g(x)$, then $If - T_k^{(0)} = O(h^{3/2})$, and the convergence of $T_k^{(0)}$ is at the same rate as the trapezoidal rule $T_0^{(k)}$. Noting this, various authors [8], [9], and [10] have suggested modifying (5) to account for the h^{α_i} terms in (6). We then get the modified Romberg quadrature, with (5) replaced by

$$\begin{aligned} \tilde{T}_k^{(m)} &= (2^{\alpha_k} \tilde{T}_{k-1}^{(m+1)} - \tilde{T}_{k-1}^{(m)})/(2^{\alpha_k} - 1), \\ \tilde{T}_0^{(k)} &= T_0^{(k)}. \end{aligned} \tag{7}$$

This modified algorithm either requires the user to supply all the α's or the code itself must try to estimate them [11].

In the case of functions with logarithmic singularities at an endpoint, the error expansion is more complicated. Thus, it is shown in [6] that if

$$\begin{aligned} f(x) &= x^\beta (1 - x)^\omega \quad \ln x h(x), \qquad \omega, \beta > -1, \\ E(h, f) &= \sum_{j=0}^{k-1} (e_j + a_j \ln h) h^{\beta+j+1} + b_j h^{\omega+j+1} + O(h^k). \end{aligned} \tag{8}$$

For the expansion (8), modifications to (5) analogous to (7) can be derived.

In an attempt to relieve the user of the need for explicitly providing the error expansion (3), (6), or (8), we allow the exponents α_i in (6) to be unknown and consider the problem of using three successive estimates to eliminate the lowest order term in the error. Thus,

$$
\begin{aligned}
(I - Q_h)f &= E(h, f) \approx a_1 h^{\alpha_1}, \\
(I - Q_{h/2})f &= E(h/2, f) \approx a_1 (h/2)^{\alpha_1}, \qquad (9)\\
(I - Q_{h/4})f &= E(h/4, f) \approx a_1 (h/4)^{\alpha_1},
\end{aligned}
$$

and

$$If \approx Q_{h/4} - (Q_{h/4} - Q_{h/2})^2/(Q_{h/4} - 2Q_{h/2} + Q_h)$$

or

$$If \approx Q_{h/4} - (\Delta Q_{h/2})^2/\Delta^2 Q_h. \qquad (10)$$

In the form (10), this is known as Aitken's del-square process. It has succeeded in eliminating the lowest order in the error term (6) at the expense of one additional trapezoidal estimate. Of course, it does not work for (8).

The difference between modified Romberg (7) and Aitken's (10) is more than just the need for a third term in (10) but rather its fundamentally nonlinear character. After one application of (7) and (10), respectively, to (6), we have

$$If - \frac{2^{\alpha_1} Q_{h/2} - Q_h}{2^{\alpha_1} - 1} \sim \hat{a}_2 h^{\alpha_2} + \hat{a}_3 h^{\alpha_3} + \cdots , \qquad (11)$$

and

$$If - [Q_{h/4} - (\Delta Q_{h/2})^2/\Delta^2 Q_h] \sim a_2' h^{\alpha_2} + O(h^{\alpha_2}); \qquad (12)$$

but (12) now contains new terms not present in the original expansion. For example, if $Q_h = h^\alpha + h^{\alpha+\beta}$, $\alpha, \beta > 0$ $(I = 0)$, one application of (7) has an error which is $O(h^{\alpha+\beta})$, while two applications will produce I exactly. On the other hand, if we apply one step of (10) to Q_h as above,

$$
\begin{aligned}
&Q_{h/4} - (\Delta Q_{h/2})^2/(\Delta^2 Q_h) \\
&\quad = \frac{h^{\alpha+\beta}}{4^\alpha}\left\{\left(1 + \frac{1}{2^\beta}\right)^2\right\} \Big/ \left[h^\beta\left\{\left(1 - \frac{1}{2^{\alpha+\beta}}\right)^2\right\} + \frac{1}{2^\alpha}\left\{\frac{1}{2^\alpha} - 2\right\}\right]. \qquad (13)
\end{aligned}
$$

For small h, this is $O(h^{\alpha+\beta})$, but the appearance of other terms (as $h^{\alpha+2\beta}$) is also seen. A second application of (10) will eliminate the $h^{\alpha+\beta}$ term, but will not be zero because of these spurious terms. Experiments with this algorithm have convinced the author that its convergence is very slow indeed [15].

An important generalization of (10), known as the ϵ-algorithm, is due to D. Shanks [12] and P. Wynn [13]. We compute $T_0^{(r+1)}$ from (1) and then $\hat{T}_1^{(r)}, \hat{T}_2^{(r-1)}, \cdots, \hat{T}_{r+1}^{(0)}$ in turn, according to

$$
\begin{aligned}
\hat{T}_k^{(m)} &= \hat{T}_{k-2}^{(m-1)} + 1/(\hat{T}_{k-1}^{(m-1)} - \hat{T}_{k-1}^{(m-2)}), \qquad (14)\\
\hat{T}_0^{(k)} &= T_0^{(k)} \quad \text{and} \quad \hat{T}_{-1}^{(k)} = 0.
\end{aligned}
$$

Let us consider $E_k(h, f)$, the error expansion (6) truncated after k terms,

$$E_k(h, f) = \sum_{t=1}^{k} a_t h^{\alpha_t}, \qquad 0 < \alpha_1 < \alpha_2 \cdots < \alpha_k. \qquad (15)$$

If the remaining terms in $E(h, f)$ are ignored, it is reasonable to try to use $2k + 1$ trapezoidal estimates to compute If by solving the $2k + 1$ nonlinear equations

(16) $$\widehat{If} - Q_{h/2^i} = E_k(h/2^i, f), \qquad i = 0, 1, \cdots, 2k.$$

Then,

$$\widehat{If} = If + O(h^{2k})$$

(Aitken's process demonstrates this for $k = 1$). The ϵ-algorithm (14) is an efficient algorithm for solving (16) for any k. Thus, if the expansion (6) actually terminates so that $E_k(h, f) = E(h, f)$, then [14]

$$\hat{T}_{2r+1}^{(0)} = If + O(h^{\alpha_{r+1}}), \qquad r = 0, 1, 2, \cdots, k - 1,$$

and, barring roundoff,

(17) $$\hat{T}_{2k+1}^{(0)} = If.$$

(The elements $\hat{T}_{2k}^{(i)}$ may be thought of as work columns.) Moreover, (14) can be used not only when E_k is obtained by truncating (6) but also for the case when E_k is the truncated expansion corresponding to a function $f(x)$ with a logarithmic singularity, as for example in (8). In order to see the truth of the last comment, it suffices to note that (17) will be true for any sequence of numbers $T_0^{(r)}$, $r = 0, \cdots, 2k + 1$, that satisfy a linear difference equation with constant coefficients [17], and that $E_k(h, f)$ for either (6) or (8) may be written as a linear combination of terms of the form

(18) $$h^{\alpha_i} = \lambda_i^m, \qquad h = 1/2^m$$

and

(19) $$(\ln h)h^{\beta_i} = m\eta_i^m, \qquad h = 1/2^m.$$

Thus,

$$E_k(h, f) = \sum_{i=1}^{k} (a_i\lambda_i^m + b_i\eta_i^m + c_i m\eta_i^m).$$

In the simpler case of (6), the stability of the ϵ-algorithm has been considered [14]. The propagation of absolute error from one odd numbered column to another is governed by a multiplicative factor of magnitude

(20) $$\sim(1/(2^{\alpha_s} - 1))^2.$$

We see that, unless there are several very high order algebraic singularities (corresponding to small α_s), such error propagation is not troublesome. On the other hand, errors in the even numbered columns can be considerable [14]. Finally, we note that the error expansions (6) and (8) require the singularity to be at an endpoint. The analogous expansions for arbitrarily located singularities are not of the same form. There is no reason to suppose that any of these algorithms will be appropriate unless the singularity is at an endpoint. In practice, this means that while the user need not specify the precise nature of the singularity, he does have to know its precise location.

3. Numerical Results. We have written a code implementing the ϵ-algorithm for quadrature, and tested it for stability and accuracy. Details of these results are described in [16]. In general, it performed about as expected. There was no large loss of accuracy in the estimates as long as reasonable precautions were taken to prevent the computation from continuing past convergence. Compared to the unmodified Romberg integration, convergence required several orders of magnitude fewer function values on integrands with the type of singularities described, but more function values than with a properly coded modified Romberg code. For smooth functions, substantially more function values were required than with the unmodified Romberg quadrature.

Our results strongly suggest that the ϵ-algorithm deserves to be considered in those applications where Romberg's method is known to converge slowly because of endpoint singularities, and modification to take such singularities into account is inconvenient. Further, this type of scheme can be built into a code that allows the *user* to specify the type of singularity if it is known, in which case he gets the more rapid convergence of the modified Romberg's method. If he cannot (or will not) specify the singularity, then the rate of convergence is still substantially better than the unmodified Romberg.

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