ON A MODIFICATION OF ROMBERG QUADRATURE

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1. Introduction. Meir and Sharma [1] have suggested a modification of Romberg quadrature using Newton-Cotes and, in particular, Simpson sums in place of trapezoidal sums. By comparing the error term with that obtained by Bulirsch [3] for trapezoidal sums, they concluded that the use of Simpson sums would lead to an improvement of the results. The procedure adopted by Meir and Sharma [1] permits them to obtain an expression for the error in the numerical quadrature. However, for the purpose of numerical computation, this procedure appears to be less suitable. In section 3, we give an alternative formulation which would enable us to carry out the computation, using Simpson sums, in the same wasy as is done in the case of Romberg quadrature with trapezoidal sums. Some numerical results are discussed in section 4.

2. For a given Riemann integrable function $f(x)$ defined on $[0, 1]$ and for a given h, $0 < h \leq 1$ with $1/h$ an integer, the trapezoidal sum $T(h)$ is given by

$$T(h) = h[\frac{1}{2} f(0) + f(h) + \ldots + \frac{1}{2} f(1)] .$$

In case of Romberg quadrature [2] we choose a sequence h_i such that $\lim_{i\to\infty} h_i = 0$ and form the sums $T(h_i) = T_o^{(i)}$. These values of $T_o^{(i)}$ for $i = 0, 1, \ldots$ are written in the first column of a triangular array. The other columns are computed from a recurrence relation

$$(2.1) \qquad T_m^{(k)} = \beta_m^{(k)} T_{m-1}^{(k)} + (1-\beta_m^{(k)}) T_{m-1}^{(k+1)}$$

where $\beta_m^{(k)} = h_{m+k}^2 / (h_{m+k}^2 - h_k^2) \quad k = 0, 1, \ldots, m-1.$

Convergence of the T_o - column and also the diagonal sequences $T_m^{(k)}$ as $m \to \infty$ to the value of the integral has been discussed in [2], while the error [3, Th.2] is given by

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$$(2.2)\qquad \int_0^1 f(x)dx - T_{m+1}^{(o)} = R_T^{(m+1)},$$

where $\quad R_T^{(m+1)} = (-1)^m B_{2m+4} f^{2m+4}(\xi)/((m+2)!)^2(2m+4)!\,.$

On the other hand, the Simpson sum $S(h)$ is given by

$$(2.3)\qquad S(h) = h[f(0) + 4f(h) + 2f(2h) \quad \ldots + f(1)]/3.$$

If we take a suitable sequence h_i as before and form the sums $S(h_i) = S_0^{(i)}$, then as in [1, eq. 28]

$$(2.4)\qquad \int_0^1 f(x)dx - \sum_{i=0}^{n} d_{ni} S_0^{(i)} = R_S^{(n)},$$

where

$$R_S^{(n)} = \frac{(-1)^n B_{2n+4}(2-2^{(-2n-1)})f^{2n+4}(\xi)}{(n+1)(n+2)(2n+3)((2n+4)!)((n+1)!)^2}.$$

Here $S_0^{(i)}$ corresponds to $N_2(h_i)$ used in [1] and $\{d_{nk}\}$ is a triangular matrix with

$$(2.5)\qquad \sum_{i=0}^{n} d_{ni} = 1 \text{ and } \sum_{i=0}^{n} d_{ni} h_i^{4+2s} = 0 \text{ for } s = 0, 1, \ldots, n-1.$$

A comparison of the expressions for $R_T^{(n+1)}$ and $R_S^{(n)}$ in (2.2) and (2.4) shows the presence of an additional factor of order $1/n$ in $R_S^{(n)}$. This indicates that for a particular magnitude of the error, use of Simpson sums would require fewer ($\simeq 1/n$th) steps. As will be seen later, much of this advantage is lost in actual computation because of the additional work involved in computing the first column of $S_0^{(i)}$ in place of $T_0^{(i)}$.

In order to estimate the value of the integral by

$$(2.6)\qquad S_n^{(0)} = \sum_{i=0}^{n} d_{ni} S_0^{(i)}$$

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we require the coefficients d_{ni} for a given n to be determined by solving the set of $(n+1)$ equations (2.5). For any other value of n these equations will have to be solved again. It is possible to solve these equations for various values of n and for a given sequence h_i once for all and tabulate them. However, from the point of view of practical computation such a procedure is not very efficient as it would require that all these numbers be first read and stored before the method is used. Alternatively, one can also write down the solutions of these equations explicitly, as will be shown later, and compute d_{ni} as and when required. Although, it is possible to write down the expressions for d_{ni} in compact form, it is easily seen from the number of multiplications required in their determination that this procedure is also not suitable.

3. Instead of solving the system (2.5) we shall develop here a procedure similar to that used in Romberg quadrature with trapezoidal sums [2]. We first compute Simpson sums $S_0^{(i)}$ for a particular sequence h_i and write it as a first column of a triangular array $S_m^{(k)}$ $(m = 0, 1, 2, \ldots, k = 0, 1, 2, \ldots)$. Every entry $S_m^{(k)}$ $(m \neq 0)$ is computed from the formula

$$(3.1) \qquad S_m^{(k)} = \alpha_m^{(k)} S_{m-1}^{(k)} + (1 - \alpha_m^{(k)}) S_{m-1}^{(k+1)} .$$

We shall show below that it is possible to determine $\alpha_m^{(k)}$ such that the algorithm described by (3.1) is equivalent to solving (2.5), to obtain $S_n^{(0)}$ from (2.6). The advantage of using (3.1) is that one can compute $S_m^{(0)}$ as well as $S_m^{(k)}$ for successive values of m and k until some desired convergence is attained.

From (2.6) we see that the value of $S_m^{(o)}$ is obtained by a linear combination of the values of $S_0^{(o)}, \ldots, S_0^{(m)}$. The coefficients d_{mi} $(i = 0, 1, \ldots, m)$ satisfy (2.5). In a similar manner we define $S_m^{(k)}$ such that

$$(3.2) \qquad S_m^{(k)} = \sum_{i=0}^{m} d_{mi}^{(k)} S_0^{(i+k)}, \quad k = 0, 1, \ldots,$$

where d_{mi} are now denoted by $d_{mi}^{(0)}$. Also $d_{mi}^{(k)}$ satisfy

$$(3.3)\quad \sum_{i=0}^{m} d_{mi}^{(k)} = 1, \quad \sum_{i=0}^{m} d_{mi}^{(k)} h_{i+k}^{4+2s} = 0 \text{ for } s = 0, 1, \ldots, m-1,$$

so that for $k = 0$ the equations (3.2) and (3.3) go over to (2.6) and (2.5). The value of $S_m^{(k)}$ is obtained by a linear combination of the values of $S_0^{(k)}, \ldots, S_0^{(k+m)}$. From equations (2.5) and (3.3) it is clear that the expressions for $d_{mi}^{(k)}$ can be written down from those of $d_{mi}^{(0)}$ by simply increasing the subscripts of each h_i appearing in $d_{mi}^{(0)}$ by k. In fact $S_m^{(k)}$ has the same interpretation as $S_m^{(0)}$ except that in case of $S_m^{(k)}$ we consider Simpson sums formed starting from $S_0^{(k)}$.

Starting from the first column $S_0^{(i)}$ of Simpson sums, we defined the elements $S_m^{(k)}$ of the triangular array by means of (3.2), where the coefficients $d_{mi}^{(k)}$ satisfy (3.3). On the other hand we have also defined $S_m^{(k)}$ by means of (3.1). We shall now show that for a proper choice of $\alpha_m^{(k)}$, the two ways of defining $S_m^{(k)}$ are consistent. From (3.1) and (3.2) we have

$$S_m^{(k)} = \sum_{i=0}^{m} d_{mi}^{(k)} S_0^{(i+k)} = \alpha_m^{(k)} S_{m-1}^{(k)} + (1 - \alpha_m^{(k)}) S_{m-1}^{(k+1)}$$

$$= \alpha_m^{(k)} \sum_{i=0}^{m-1} d_{m-1,i}^{(k)} S_0^{(i+k)} + (1 - \alpha_m^{(k)}) \sum_{i=0}^{m-1} d_{m-1,i}^{(k+1)} S_0^{(i+k+1)}.$$

Comparing the coefficients of $S_0^{(i+k)}$ for $i = 0, 1 \ldots, m$ we get

$$d_{m,0}^{(k)} = \alpha_m^{(k)} d_{m-1,0}^{(k)},$$

$$(3.4)\quad d_{m,j}^{(k)} = \alpha_m^{(k)} d_{m-1,j}^{(k)} + (1 - \alpha_m^{(k)}) d_{m-1,j-1}^{(k+1)} \qquad j = 1, \ldots, m-1.$$

$$d_{m,m}^{(k)} = (1 - \alpha_m^{(k)}) d_{m-1,m-1}^{(k+1)}.$$

Assuming now that $d_{m,i}^{(k)}$, $d_{m-1,i}^{(k)}$ and $d_{m-1,i}^{(k+1)}$ $(i = 0, 1, \ldots)$

satisfy (3.3), if we can determine a value of $\alpha_m^{(k)}$ which will satisfy all the $(m+1)$ equations (3.4) our assumption (3.1) will be justified. This will also determine the required value of $\alpha_m^{(k)}$.

By using Cramer's rule the solution of the equations (3.3) can be written down explicitly as

$$(3.5) \qquad d_{m,r}^{(k)} = \prod_{i=0}^{m} h_{k+i}^2 / [h_{k+r}^4 \sum_{i=0}^{m} (1/h_{k+i}^2) \prod_{\substack{i=0 \\ i\neq r}}^{m} (h_{k+i}^2 - h_{k+r}^2)]$$

$$r = 0, 1, \ldots, m.$$

From the first equation (3.4) using (3.5) we get

$$(3.6) \quad \alpha_m^{(k)} = d_{m,0}^{(k)} / d_{m-1,0}^{(k)} = h_{k+m}^2 \sum_{i=0}^{m-1} (1/h_{k+i}^2) / [(h_{k+m}^2 - h_k^2) \sum_{i=0}^{m} 1/h_{k+i}^2]$$

It is now a matter of straightforward but tedious calculations to verify that the remaining equations (3.5) are satisfied for the same value of $\alpha_m^{(k)}$. This completes the proof. Note that we can also write

$$\alpha_m^{(k)} = \beta_m^{(k)} \sum_{i=0}^{m-1} h_{k+1}^{-2} / (\sum_{i=0}^{m} h_{k+i}^{-2}).$$

Where $\beta_m^{(k)}$ is the same as in (2.1). It is clear that $|\alpha_m^{(k)}| < |\beta_m^{(k)}|$ and for large m we have $\alpha_m^{(k)} \simeq \beta_m^{(k)}$.

4. Numerical results. Three different sequences for h_i have been considered. These sequences are chosen in such a way that the number of points (i.e. $1/h_i$) increases rapidly, moderately and slowly. In the case when the number of points increases very rapidly, the amount of computation involved in calculating the first column increases. On the other hand, for those sequences for which the number of points increases very slowly, there is the danger of round-off errors accumulating. Various integrals have been evaluated using Simpson sums and the algorithm given in (3.1). The same integrals have also been evaluated using trapezoidal sums and similar sequences.

In the following $\mathcal{T}$ denotes a particular sequence $\{h_i\}$ and f_m denotes the number of function evaluations required to compute the first column up to $S_0^{(m)}$ for a given m.

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Sequence $\mathfrak{F}_1$: $h_i = 1/2^{(i+1)}$ $i = 1, 2, \ldots$

m	0	1	2	3	4	5	6
f_m	3	5	9	17	33	65	129

Sequence $\mathfrak{F}_2$:

$$h_i = \begin{cases} 1/2^{(i+4)/2} & i = 0, 2, 4, \ldots \\ 1/3 \cdot 2^{(i+1)/2} & i = 1, 3, 5, \ldots \end{cases}$$

m	0	1	2	3	4	5	6	7	8	9	10
f_m	5	9	13	17	25	33	49	65	97	129	193

Sequence $\mathfrak{F}_3$: $h_i = 1/2(i+1)$ $i = 0, 1, 2, \ldots$

m	0	1	2	3	4	5	6	7	8	9	10	11	12	13
f_m	3	5	9	13	21	25	37	45	57	65	85	93	117	129

Various integrals such as

i) $\int_0^{\pi/2} \sin x \, dx$, ii) $\int_0^{\pi} x \cos 3x \, dx$, iii) $\int_0^1 2x \, dx$,

iv) $\int_0^1 x^{24} \, dx$, v) $\int_0^{\infty} (1/[(1+x^2)(4+x^2)]) \, dx$,

vi) $\int_0^{\pi} \tan^{-1}\{((1/2)\sin x)/ (1-(1/2) \cos x) \} . (1/\sin x) \, dx.$

have been computed using double precision on IBM 7040. On the basis of these calculations, it was found that the problem of round-off error was not serious in using any of the sequences, although, as was expected, the round-off errors show up for the sequence $\mathfrak{F}_3$. Similarly, for a given order of accuracy, $\mathfrak{F}_1$ requires more function evaluations. $\mathfrak{F}_2$ therefore appears to be a better choice.

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The same integrals have also been evaluated using trapezoidal sums and sequences

$\mathfrak{F}_4$: $h_i = 1/2^i$ $i = 0, 1, 2, \ldots$

$\mathfrak{F}_5$: $h_i = \begin{cases} 1 & i = 0 \\ 1/2^{(i+1)/2} & i = 1, 3, 5, \ldots \\ 1/3 \cdot 2^{(i-2)/2} & i = 2, 4, 6, \ldots \end{cases}$

$\mathfrak{F}_6$: $h_0 = 1$ and $h_i = 1/2i$ $i = 1, 2, \ldots$

Naturally, for a given m the results using Simpson sums are more accurate as was expected. However, this way of comparing the two procedures is not satisfactory, because, depending upon the complexity of the function, most of the computing time could be spent in evaluating the function at various points and also in calculating the first column. If we take this aspect into consideration, we find that there is still some slight advantage in using Simpson sums over trapezoidal sums, provided it is known that the function to be integrated is sufficiently smooth and the basic assumption that the error $S(h) - I$ is $0(h^4)$ is satisfied. Sometimes the trapezoidal rule gives better results because the error is $0(h^2)$ and the function may not be sufficiently smooth [see 2, p. 213]. Finally, for certain integrals such as v) and vi) above, the convergence was very slow both in case of trapezoidal and Simpson sums.

Based on these and other [4] computations, one can say that the advantage in using Simpson sums is not so great as it may appear from the error analysis. Regarding convergence, there is no evidence that the use of Simpson sums improves the situation in any way. However, when the time required for the evaluation of the function is of importance, there is some advantage gained in using Simpson sums.

REFERENCES

1. A. Meir and A. Sharma, On the method of Romberg quadrature. J. SIAM Numer. Anal. (Ser. B) 2 (1965) 250-258.

2. F. L. Bauer, H. Rutishauser and E. Stiefel, New aspects in numerical quadrature. Proc. symp. in Appl. Math. 15 (Amer. Math. Soc., 1963) 199-218.

3. R. Bulirsch, Bemerkungen zur Romberg-Integration. Num. Math. 6 (1964) 6-16.

https://doi.org/10.4153/CMB-1968-025-x Published online by Cambridge University Press

4. C. Turnbull, A study of some methods of numerical quadrature. Master's Thesis (Univ. of Saskatchewan, Saskatoon, 1967).

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