

# Error estimation in the Clenshaw–Curtis quadrature formula

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Several error estimates for the Clenshaw–Curtis quadrature formula are compared. Amongst these is one which is not unrealistically large, but which is easy to compute and reliable when certain conditions are satisfied. The form of this new error estimate helps explain the considerable accuracy of the Clenshaw–Curtis method when the integrand is well behaved; in this case the method is nearly as accurate as Gaussian quadratures. It is argued that the Clenshaw–Curtis method is a better method for evaluating such integrals than either Romberg's process or Gaussian quadratures.

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## 1. Introduction

Clenshaw and Curtis (1960) have described a method for evaluating a definite integral by expanding the integrand in a finite Chebyshev series and integrating the terms in the series one by one. This has been shown in practice to be an efficient method for evaluating integrals because of the accuracy and simplicity of the method, and because of the ease with which it is possible to estimate the error (Clenshaw and Curtis, 1960; Fraser and Wilson, 1966; Wright, 1966; Kennedy and Smith, 1967).

Two methods for estimating the error have been given by Clenshaw and Curtis but these usually give rise to conservative error estimates. In this paper we compare these with some new error estimates one of which,  $|E_N^{(\varphi)}|$ , is a close error bound and reliable when the conditions in equations (13) and (14) are satisfied. We attempt an explanation why the Clenshaw–Curtis method gives results nearly as accurate as Gaussian quadratures for the same number of abscissae.

In the last section we give some examples which support the view that, in general, the Clenshaw–Curtis method is a more efficient method for evaluating integrals than Gaussian quadratures or Romberg's process.

In the following we will always assume that the computer word length is large enough that rounding errors are negligible.

## 2. Theory

In the method of Clenshaw and Curtis the interval of integration is first changed to  $(-1, +1)$  and the integral written in the form

$$I = \int_{-1}^1 F(t) dt. \quad (1)$$

The function  $F(t)$  is approximated by a finite Chebyshev series

$$F(t) = \sum_{r=0}^N a_r T_r(t) \quad (2)$$

where  $\Sigma''$  denotes a finite sum whose first and last terms are to be halved. The coefficients  $a_r$  are calculated from the equation

$$a_r = \frac{2}{N} \sum_{s=0}^N \cos \frac{\pi r s}{N} F\left(\cos \frac{\pi s}{N}\right) \quad (3)$$

and the series in (2) is integrated term by term. It has been shown (Imhof, 1963; Smith, 1962 and 1965) that this process of Clenshaw and Curtis is equivalent to a quadrature formula

$$I_N = \sum_{s=0}^N h_s^{(N)} F\left(\cos \frac{\pi s}{N}\right) \quad (4)$$

where the weights  $h_s^{(\Lambda)}$  are given by

$$h_s^{(N)} = \frac{2(-1)^s}{N^2 - 1} + \frac{4}{N} \sin \frac{s\pi}{N} \sum_{i=1}^N \frac{\sin [(2i - 1)s\pi/N]}{2i - 1} \quad (5)$$

for  $1 \leq s \leq N - 1$ ,

$$h_0^{(N)} = h_N^{(N)} = (N^2 - 1)^{-1}. \quad (6)$$

Some of these weights have been given by Fraser and Wilson (1966) but they are easily computed to any accuracy at the beginning of a computer program for the values  $N$  needed.

If the integrand  $F(t)$  is expanded in an infinite Chebyshev series

$$F(t) = \sum_{r=0}^{\infty} A_r T_r(t) \quad (7)$$

where  $\Sigma'$  denotes a sum whose first term is to be halved, the error  $E_N = I - I_N$  is given by

$$E_N = \sum_{r=0}^{\frac{1}{2}N-1} \frac{2A_{2N-2r}}{4r^2 - 1} + \sum_{r=0}^{\frac{1}{2}N-1} \frac{2A_{2N+2r}}{4r^2 - 1} - \sum_{r=1}^{N-1} \frac{2A_{N+2r}}{(N+2r+1)(N+2r-1)} \quad (8)$$

in which we have assumed that  $N$  is even and that terms equal to and higher than  $A_{3N}$  are negligible. By combining the first and second summations Clenshaw and Curtis obtained one of their error estimates (we will discuss this later), but by combining all three summations considerable cancellation occurs, especially in the first and third summations, with the result that  $E_N$  takes the simpler form:

$$E_N = \frac{16.1 \cdot N}{(N^2 - 1^2)(N^2 - 3^2)} A_{N+2} + \frac{16.2 \cdot N}{(N^2 - 3^2)(N^2 - 5^2)} A_{N+4} + \dots$$

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$$\begin{aligned}
 &+ \frac{16(N/2 - 1)N}{3(2N - 1)(2N - 3)} A_{2N-2} \\
 &- \left(2 + \frac{2}{4N^2 - 1}\right) A_{2N} \\
 &+ \left(\frac{2}{3} - \frac{2}{(2N + 1)(2N + 3)}\right) A_{2N+2} + \dots \quad (9)
 \end{aligned}$$

This new form for the error gives us some insight into the accuracy of the Clenshaw–Curtis formula: because of the fast convergence of the Chebyshev series, the first Chebyshev coefficients  $A_{N+2}$ ,  $A_{N+4}$ , etc., are the largest in (9) but the factors of these first coefficients, of order  $1/N^3$ , are the smallest. The scalar product of the factors and coefficients is therefore a sum over a number of small terms.

It is interesting to note that the result thus obtained with the approximate Chebyshev coefficients  $a_r$  is better than that which would be obtained by integrating the finite Chebyshev series with the exact Chebyshev coefficients  $A_r$ . The coefficients  $a_r$  effectively take cognisance of the ‘higher harmonics’ and eliminate a major part of the error due to them. Hence the Clenshaw–Curtis method has an accuracy considerably higher than order  $N$  and usually has an error not much larger than that obtained with Gaussian quadratures. This result is true for both well behaved and badly behaved functions (we define a well behaved function as one whose Chebyshev coefficients  $A_r$  converge quickly).

### 3. Error estimates

#### 3.1. The Clenshaw–Curtis error estimates

Clenshaw and Curtis have suggested two methods for estimating the error. In the first it is assumed that the Chebyshev expansion for  $F(t)$  converges quickly. The indefinite integral

$$I(x) = \int_{-1}^x \left[ \sum_{r=0}^N a_r T_r(t) \right] dt$$

is written as a Chebyshev series with coefficients  $b_r$ , and for the definite integral,  $x = 1$ , the largest of  $b_{N+1}$ ,  $kb_{N-1}$  and  $k^2b_{N-3}$  is chosen as an error estimate, where  $k$  is a constant which they suggest should be taken as  $1/8$ . Three independent numbers are used to estimate the error in case one or two should be accidentally small. This is equivalent to choosing as the error estimate

$$\begin{aligned}
 E_N^{(1)} = \max &\left[ \frac{|a_N|}{4(N+1)}, \frac{1}{32(N-1)} |2a_{N-2} - a_N|, \right. \\
 &\left. \frac{1}{128(N-3)} |a_{N-4} - a_{N-2}| \right]
 \end{aligned}$$

where the quantities  $a_r$  are computed using equation (3) or using the simpler form:

$$a_{N-2r} = \frac{2}{N} \sum_{s=0}^N (-1)^s F\left(\cos \frac{s\pi}{N}\right) \cos \frac{2rs\pi}{N}. \quad (10)$$

When the Chebyshev expansion for  $F(t)$  is slowly convergent Clenshaw and Curtis assume that coefficients higher than  $A_{3N}$  can be neglected and that between  $A_{N+2}$  and  $A_{3N}$  the coefficients satisfy an inequality of the form  $|A_r| \leq K_N/r$ . By combining the first and second summations in (8) they show that  $|E_N| < 2K_N/N$ . The largest of  $|a_N|$ ,  $2|a_{N-2}|$  and  $2|a_{N-4}|$  is then used to estimate  $2K_N/N$ . We call this  $E_N^{(2)}$ .

We now look at the series in (8) and (9) again, and deduce some other estimates.

#### 3.2. Error estimate (a)

We begin by noting that for most regular functions the convergence of the Chebyshev series is rapid; indeed, in general,  $|A_r|$  falls to zero exponentially as  $r$  increases to infinity (Elliott, 1964). Therefore, the first term in the series for  $E_N$  in equation (9) is often larger than the sum of the other terms. For example, if we define  $|A_{2r}|$  in terms of  $|A_{N+2}|$  using the recurrence relation  $|A_{r+2}| = K_N|A_r|$ , then a simple calculation shows that the first term equals the absolute sum of the other terms for the values of  $K_N$  given in Table 1. Therefore, the

Table 1  
Values of  $K_N$  defined in equation (11)

$N$	4	6	8	12	16	24
$K_N$	0.28	0.12	0.14	0.21	0.24	0.28
$N$	32	48	64	96	128	192
$K_N$	0.28	0.28	0.29	0.29	0.29	0.29

first term dominates the series in (9) when

$$|A_{r+2}/A_r| < K_N \text{ for } r > N + 2. \quad (11)$$

This criterion is usually satisfied by analytic functions if there is no singularity close to the real axis between  $-1$  and  $+1$  (see, for example, the tables of Chebyshev coefficients given by Clenshaw (1962)). In the case of such a well behaved function twice the first term is an error bound

$$|E_N| < \frac{32N}{(N^2 - 1)(N^2 - 9)} |A_{N+2}|.$$

(It is worth noting that the asymptotic behaviour of this error,  $E_N \sim O(\sum A_r/N^3)$ , is in agreement with that obtained by Elliott (1965) using complex variable theory.) Since in general  $|A_{N+2}| < A_N = \frac{1}{2}|a_N|$ , we can replace  $|A_{N+2}|$  by  $\frac{1}{2}|a_N|$ , but because of the possibility that  $|a_N|$  might be accidentally small we use as our error estimate

$$|E_N^{(a)}| = \frac{16N}{(N^2 - 1)(N^2 - 9)} \max [ |a_N|, 2k|a_{N-2}|, 2k^2|a_{N-4}| ] \quad (12)$$

where we suggest, because of (11), that  $k$  is taken to be  $\frac{1}{4}$  except when  $N = 6$  and  $N = 8$ . This estimate shows why Wright (1966) found empirically that the error varied as  $a_N/N^3$ .

The error estimate in (12) is reliable for well behaved functions, but it must be used with care. It is not difficult to find rapidly varying functions for which  $|E_N^{(a)}|$  is not a bound to  $E_N$ . For example, if  $F(t)$  has a discontinuity  $\Delta F$  at  $t = a$  then it is easily shown that

$$A_r = \frac{2}{\pi r} \Delta F \sin(ra) + \frac{2}{\pi r} \int_0^{\pi} F'(\cos \theta) \sin r\theta \sin \theta d\theta;$$

so  $|A_r|$  falls to zero at a rate  $1/r$ . Similarly if  $F(t)$  is continuous but  $F'(t)$  is discontinuous then  $|A_r|$  falls off at a rate  $1/r^2$ . Worst of all, if  $F(t)$  is a delta function the coefficients  $A_r$  have no limit; they oscillate between a maximum and minimum value for all  $r$ . Even if  $F(t)$  and all its derivatives are continuous it may change rapidly at some point in the interval (perhaps due to a pole just off the real axis) and it may then be approximated by a function containing a delta function or a discontinuity. In this case the behaviour of  $A_r$  for small (practical) values of  $r$  will be like that for the approximate function and the error estimate  $|E_N^{(a)}|$  is liable to failure.

To guard against this failure we suggest the following checking procedure. As we have shown in Table 1 the first term in the series dominates the error expansion in equation (9) if  $|A_{r-2}/A_r|$  is less than about  $k = \frac{1}{4}$ , for  $r \geq N + 2$ . We do not know these coefficients but we can reasonably assume that the rate at which they are decreasing is similar to the rate at which the last four coefficients  $|a_r|$  are falling towards zero. Therefore we check that

$$\frac{1}{2}|a_N| < k|a_{N-2}| < k^2|a_{N-4}| < k^3|a_{N-6}| \quad (13)$$

where we suggest  $k$  is taken to be  $\frac{1}{4}$ . As a further check we note that  $|I_N - I_{N/2}|$  should be a good error estimate for the quadrature  $I_{N/2}$  if the coefficients are falling quickly. Therefore we check that

$$|E_{N/2}^{(a)}| > |I_N - I_{N/2}|. \quad (14)$$

Only if these four inequalities are satisfied do we accept  $|E_N^{(a)}|$ .

### 3.3. Error estimate (b)

If the estimate (a) fails either another estimate or a different method must be used to evaluate the integral. Let us assume that we know the function is continuous with no sharp peaks; then at worst the coefficients  $A_r$  fall off as  $1/r^2$ . We write  $A_r = K_N/r^2$  for  $r \geq N$  and sum the right-hand side of equation (9) to infinity. Then putting

$$\frac{1}{2}|a_N| = (K_N/N^2)[1 + 3^{-2} + 5^{-2} + \dots]$$

we find a new error estimate

$$|E_N^{(b)}| < C_N|a_N| \quad (15)$$

where  $C_N$  is a function of  $N$  only. The values of  $C_N$  given in Table 2 show that  $C_N$  is close to  $\frac{2}{3}$  for most values of  $N$ . As in equation (12) we use  $|a_{N-2}|$ ,  $|a_{N-4}|$  and (for reasons we explain in the appendix)  $|I_N - I_{N/2}|$

Table 2

Coefficients $C_N$ appearing in the error estimate $ E_N^{(b)} $							
$N$	4	8	16	32	64	128	256
$C_N$	0.586	0.628	0.646	0.654	0.658	0.660	0.662

in case  $|a_N|$  is accidentally small. So our error estimate (b) has the form

$$|E_N^{(b)}| = C_N \max [|a_N|, 2|a_{N-2}|, |I_N - I_{N/2}|]. \quad (16)$$

This is very similar to the error estimate  $|E_N^{(2)}|$  of Clenshaw and Curtis. It has the advantage, however, that we can easily add a check that it is probably a bound. In its derivation we assumed that  $A_r$  fell off at least as fast as  $1/r^2$ . This suggests the condition

$$\frac{N^2}{2}|a_N| < (N-2)^2|a_{N-2}| < (N-4)^2|a_{N-4}| < (N-6)^2|a_{N-6}| \quad (17)$$

and the further condition

$$|I_N - I_{N/2}| < |E_{N/2}^{(b)}|. \quad (18)$$

### 3.4. Error estimate (c)

Another error estimate, similar to this, can be obtained by comparing  $I_N$  with the integration formula derived by expanding  $F(t)$  in a Chebyshev series of the second kind:

$$F(t) = \sum_{r=0}^{N-2} C_r U_r(t).$$

Following the derivation of (4) with  $T_r(x)$  replaced by  $U_r(x)$  we obtain a new quadrature formula ( $N$  even)

$$I'_N = \sum_{s=1}^{N-1} \omega_s F\left(\cos \frac{\pi s}{N}\right)$$

where

$$\omega_s = \frac{4}{N} \sin \frac{s\pi}{N} \sum_{j=1}^{\frac{1}{2}N} \frac{\sin [(2j-1)s\pi/N]}{2j-1}.$$

This formula is effectively the same as that described by Fillipi (1964). It bears an interesting relation with the Clenshaw-Curtis formula, for the difference between the two has the simple form:

$$|I_N - I'_N| = \frac{N}{N^2 - 1} |a_N|. \quad (19)$$

This and the result in (9) shows why  $I'_N$  is usually less accurate than  $I_N$ , a result found in practice by Wright (1966).

Since the two quadrature formulae  $I_N$  and  $I'_N$  fit different orders of polynomials to different points (the Clenshaw-Curtis formula includes the end points; the formula based on the polynomials  $U_r(t)$  does not) they are independent and the expression in equation (19) can be used to estimate the accuracy of  $I_N$ . We call this error estimate  $|E_N^{(c)}|$ . It is related to the Clenshaw-Curtis estimate  $|E_N^{(b)}|$ , since to a good approximation  $|E_N^{(c)}| = 4|E_N^{(b)}|$ . The similarity between the two estimates clearly arises because, as is readily shown, the

derivations of the two estimates are not independent. The error  $|E_N^{(\phi)}|$  has been used with great effect and reliability by Kennedy and Smith (1967) in some recent physical calculations, but because conditions for its use are not as clearly defined as for the previous two error estimates  $|E_N^{(\psi)}|$  and  $|E_N^{(\phi)}|$ , we feel the latter two are probably better in most cases.

3.5. Comparison of error estimates

The error estimates  $|E_N^{(\psi)}|$ ,  $|E_N^{(\phi)}|$ ,  $|E_N^{(\phi)}|$  and the Clenshaw-Curtis estimates  $|E_N^{(\psi)}|$ ,  $|E_N^{(\phi)}|$  are compared in Table 3 for four integrals which are typical of those we have tested. Estimates which are not bounds to the error are underlined.

An examination of the table shows that there is not a great deal of difference between the different estimates, except that  $|E_N^{(\psi)}|$  is a closer bound than the others for well behaved integrands when  $N$  is large.

As we have already explained this error and  $|E_N^{(\phi)}|$  have the advantage that we have specified the conditions (13) with (14) and (17) with (18) respectively which should be satisfied before these errors are accepted as bounds. We tested these on a large number of integrals by introducing a parameter  $\beta$  and by changing the variable of integration in (1) from  $t$  to  $x$  where

$$t = \frac{(\beta + 1)x + \beta - 1}{(\beta - 1)x + \beta + 1} \tag{20}$$

The integral can then be put in the form

$$I = \int_{-1}^1 F(t)dt = \int_{-1}^1 g(\beta, x)dx. \tag{21}$$

We let  $\beta$  take 100 values between 0.5 and 1.5; this allowed us to test the above conditions on 100 different (though similar) integrals for each function  $F(t)$ . Seventeen different integrands  $F(t)$  were chosen, those in Tables 3 and 4 and the following:

$$\int_0^1 e^x dx; \int_0^1 \frac{dx}{1 + 25x^2}; \int_0^{\pi/2} \frac{dx}{1 + \cos x}; \int_0^{\pi} \frac{dx}{5 + 4 \cos x};$$

$$\int_0^1 \frac{4dx}{1 + 256(x - \frac{3}{8})^2}; \int_0^1 \sqrt{x} dx; \int_0^1 \frac{dx}{1 - 0.998x^4};$$

$$\int_0^6 \phi(x)dx; \int_0^1 \psi(x)dx; \int_0^{(5/4)^3+1} (x - \frac{3}{4}(x - 1)^{1/3})dx;$$

$$\int_0^{\pi} x \cos^2 20x dx$$

where

$$\phi(x) = \begin{cases} e^x, & x \leq \frac{1}{2}; \\ e^{1-x}, & x > \frac{1}{2}; \end{cases} \text{ and } \psi(x) = \begin{cases} e^x, & x < \frac{1}{2}; \\ \frac{1}{2}(1 + e^{1/2}), & x = \frac{1}{2}; \\ e^{x-1/2}, & x > \frac{1}{2}. \end{cases}$$

Of these seven might be called 'well behaved' and the rest 'badly behaved'.

The error estimates and accompanying conditions were checked automatically on these functions for  $N = 4, 8, 16, 32$  and  $64$  (when rounding errors were not dominant) which, in all, amounted to several thousand tests. The results obtained were as follows:

(1) Out of 6505 tests,  $|E_N^{(\psi)}|$  failed to be an error bound on 3416 occasions, but the conditions (13) and (14) detected this failure in 3404 occasions and failed only on 12 occasions all for the extreme example

Table 3

Error estimates for Clenshaw-Curtis quadrature

	$N$	ERROR	$ E_N^{(\psi)} $	$ E_N^{(\phi)} $	$ E_N^{(\phi)} $	$ E_N^{(\psi)} $	$ E_N^{(\phi)} $
$\int_0^1 \frac{dx}{1+x}$	4	0.993(-5)	0.536(-2)	0.141(-1)	0.539(-1)	0.244(-1)	0.236(-1)
	8	0.640(-9)	0.929(-6)	0.123(-2)	0.566(-5)	0.227(-4)	0.973(-5)
	16	0.209(-14)	0.268(-12)	0.920(-9)	0.234(-12)	0.413(-9)	0.361(-11)
$\int_0^1 \frac{dx}{1-0.5x^4}$	4	0.103(-2)	0.865(-2)	0.245(1)	0.932(-1)	0.137(0)	0.408(-1)
	8	0.936(-5)	0.405(-4)	0.427(-1)	0.197(-3)	0.515(-2)	0.339(-3)
	16	0.103(-8)	0.249(-7)	0.498(-4)	0.126(-7)	0.542(-5)	0.195(-6)
	32	0.114(-14)	0.174(-13)	0.673(-10)	0.207(-14)	0.667(-8)	0.132(-12)
$\int_0^1 \frac{dx}{1+100x^2}$	4	0.965(-2)	0.265(-2)	0.438(0)	0.355(-1)	0.136(0)	0.156(-1)
	8	0.310(-3)	0.433(-3)	0.530(-1)	0.115(-2)	0.121(-1)	0.198(-2)
	16	0.142(-6)	0.646(-5)	0.818(-3)	0.179(-5)	0.528(-3)	0.276(-4)
	32	0.356(-10)	0.168(-8)	0.982(-6)	0.109(-9)	0.488(-6)	0.694(-8)
$\int_{-1}^1 ( x + \frac{1}{2} )^{1/2} dx$	4	0.627(-1)	0.116(-1)	0.323(1)	0.123(0)	0.152(0)	0.538(-1)
	8	0.161(-1)	0.698(-3)	0.694(-1)	0.186(-2)	0.436(-1)	0.319(-2)
	16	0.645(-2)	0.118(-3)	0.238(-1)	0.326(-4)	0.620(-2)	0.504(-3)
	32	0.213(-2)	0.226(-4)	0.415(-2)	0.147(-5)	0.283(-2)	0.931(-4)

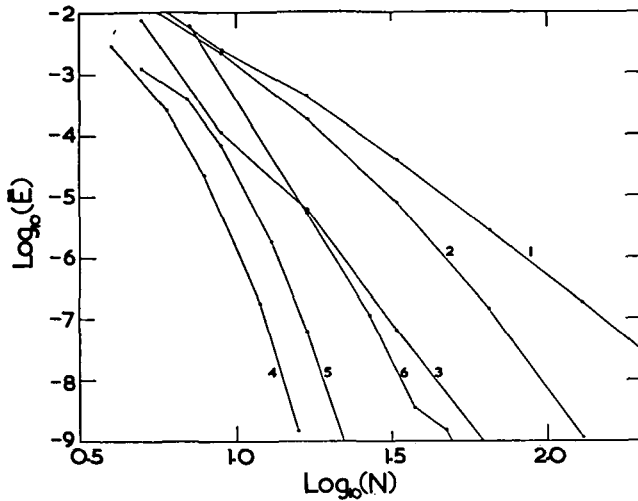


Fig. 1. A comparison of the root mean square error,  $\bar{E}$ , obtained in evaluating 100 integrals based on  $F(t) = (1 - 0.5t^4)^{-1}$  and  $0 \leq t \leq 1$ —see the text for details—by the methods: 1. Simpson's rule (equal intervals); 2. Romberg's method; 3. The (7-8) rule; 4. Gaussian quadrature; 5. Clenshaw-Curtis method; 6. Interval subdivision. The integer  $N$  is the number of function evaluations.

$\int_0^\pi x \cos^2 20x dx$  for  $N = 4$ . This shows that the use of only 5 abscissas cannot be recommended for the evaluation of an integral without additional information.

(2) Out of 4140 tests,  $|E_N^{(b)}|$  failed to be an error bound on 641 occasions, and the conditions (17) and (18) failed to locate 23 of these, a few times each for 4 of the badly behaved functions.

Thus we conclude that  $|E_N^{(b)}|$ , in conjunction with conditions (13) and (14), is a reliable method of estimating the Clenshaw-Curtis quadrature error for  $N \geq 8$ . When these conditions are not satisfied we can use  $|E_N^{(b)}|$  along with conditions (17) and (18), but not with any great reliability because as our examples show these conditions occasionally fail. We therefore recommend that if conditions (13) and (14) are not satisfied the integral should be evaluated by subdividing the range of integration and using low order quadratures in each subinterval (Wright, 1966).

There is always the possibility that the conditions (13) and (14) might fail, although we found no such cases. When extra reliability is required it is therefore advisable to demand an accuracy of an extra figure or two more than that required. For example,  $N$  could be increased till  $|E_N^{(b)}| < \epsilon/10$ , where  $\epsilon$  is the tolerated error. This would reduce the probability that  $|E_N^{(b)}| < |E_N|$  by about a factor  $10^3$ , since  $|E_N^{(b)}|$  is the largest of three nearly independent calculations—see equation (12).

#### 4. Comparison of quadrature formulas

We have compared the accuracy of a number of methods of integration with the Clenshaw-Curtis method. In previous comparisons of this kind in the literature single functions were used. Because of the

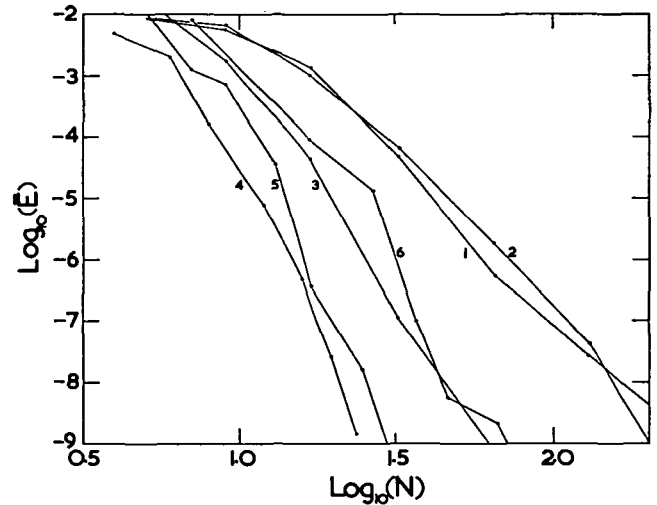


Fig. 2. As in Fig. 1, with  $F(t) = (1 + 100t^2)^{-1}$  and  $0 \leq t \leq 1$ .

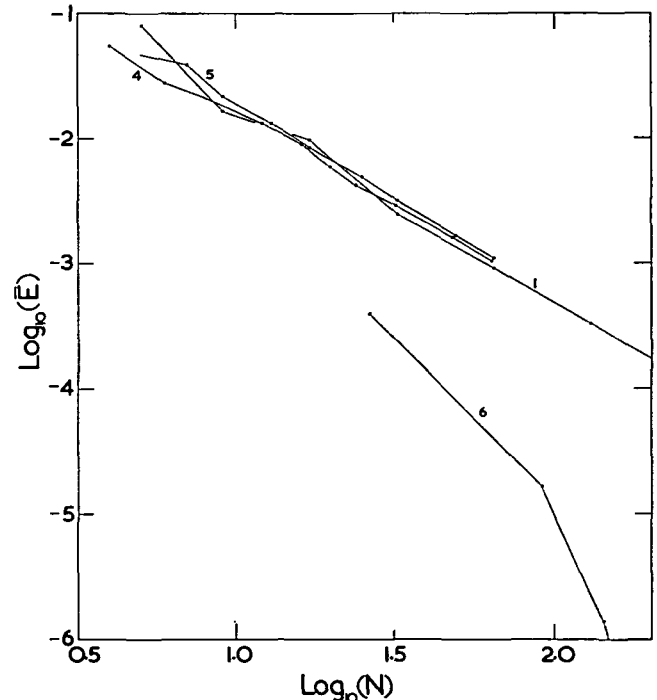


Fig. 3. As in Fig. 1, with  $F(t) = |t + \frac{1}{2}|^{1/2}$  and  $-1 \leq t \leq 1$ ; lines (2) and (3) are not shown because they lie close to lines (1), (4) and (5).

possibility that a particular function might be a special case we adopted the process, already described, in which the variable of integration is changed from  $t$  to  $x$  as in equations (20) and (21). The quadrature formula  $I_N$  is then a function of  $\beta$  and has the form

$$I_N(\beta) = \sum_i \omega_i g(\beta, x_i) \quad (22)$$

where  $\omega_i$  and  $x_i$  are the weights and abscissas of the quadrature formula concerned. We evaluated the quadratures for a hundred values of  $\beta$  between 0.5 and 1.5 for each function and we use the root-mean-square

error as an estimate of the accuracy of the quadrature method for that function. Results for three typical cases are shown in graphical form in Figs. 1, 2 and 3. (The lines joining the points have no special significance: they simply link together points for one quadrature formula.) Amongst the methods compared are Simpson's rule, Romberg's method (Romberg, 1955), the 7–8 rule (Smith, 1965), Gaussian quadratures and a method based on interval subdivision and a low order Clenshaw–Curtis quadrature in which the abscissas are concentrated near any irregularity in the function. This will shortly be published (O'Hara and Smith, 1968).

It is clear from these examples (and many others) that (1) the Clenshaw–Curtis method is much more accurate than Romberg's process for a well behaved function—it is regularly two, three or four figures more accurate; (2) it is nearly as accurate as Gaussian quadratures, but

it has the advantage that error estimates are easily calculated and that little work is lost when the number of abscissas is doubled; and (3) a method of interval subdivision is the most satisfactory if the integrand is badly behaved. We argue therefore that the Clenshaw–Curtis quadrature and error estimate  $|E_N^{(p)}|$  should be generally adopted for the evaluation of integrals provided that the integrals satisfy the conditions in equations (13) and (14).

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### References

- CLENSHAW, C. W. (1962). Chebyshev Series for Mathematical Functions, *Math. Tables*, Vol. 5, H.M.S.O., London.
- CLENSHAW, C. W., and CURTIS, A. R. (1960). A method for numerical integration on an automatic computer, *Num. Math.*, Vol. 2, pp. 197–205.
- ELLIOTT, D. (1964). The evaluation and estimation of the coefficients in the Chebyshev series expansion of a function, *Math. Comp.*, Vol. 18, pp. 274–284.
- ELLIOTT, D. (1965). Truncation errors in two Chebyshev Series Approximations, *Math. Comp.*, Vol. 19, pp. 234–248.
- FILIPPI, S. (1964). Angenäherte Tschebyscheff-Approximation einer Stammfunktion—eine Modifikation des Verfahrens von Clenshaw and Curtis, *Num. Math.*, Vol. 6, p. 320.
- FRASER, W., and WILSON, M. W. (1966). Remarks on the Clenshaw–Curtis quadrature scheme, *SIAM Review*, Vol. 8, pp. 322–327.
- IMHOF, J. P. (1963). On the method for numerical integration of Clenshaw and Curtis, *Num. Math.*, Vol. 5, p. 138.
- KENNEDY, M. (1966). M.Sc. dissertation, Queen's University, Belfast.
- KENNEDY, M., and SMITH, F. J. (1967). The evaluation of the JWKB phase shift, *Mol. Phys.* Vol. 13, pp. 443–448.
- O'HARA, H., and SMITH, F. J. (1968). Integration by sub-dividing the interval (to be published).
- ROMBERG, W. (1955). Vereinfachte numerische Integration, *Det. Kong. Norske Vid. Sel. Forh.*, Vol. 28, pp. 30–36.
- SMITH, F. J. (1962). Thesis, Queen's University, Belfast, p. 154.
- SMITH, F. J. (1965). Quadrature methods based on the Euler–MacLaurin formula and on the Clenshaw–Curtis method of integration, *Num. Math.*, Vol. 7, pp. 406–411.
- WRIGHT, K. (1966). Series methods for integration, *Computer Journal*, Vol. 9, pp. 191–199.

### Appendix

The difference  $|I_N - I_{N/2}|$  can always be used as an error estimate for any quadrature formula. Unfortunately it is well known that such estimates often fail. In practice, however, for the Clenshaw–Curtis method  $|I_N - I_{N/2}|$  is found to be close in magnitude to  $|a_N|$  and to  $|a_{N-2}|$ , especially if the integrand is badly behaved. Examples can be found by examining the tables of results given by Fraser and Wilson (1966). A large number of other examples have been given by Kennedy (1967). An explanation can be found by writing  $I_N - I_{N/2}$  in terms of the coefficients  $A_r$ , using equation (9), i.e.

$$I_N - I_{N/2} = 2 \left[ A_{N/2+2} \left( \frac{1}{(N/2-2)^2-1} - \frac{1}{(N/2+2)^2-1} \right) + A_{N/2} + 4 \left( \frac{1}{(N/2-4)^2-1} - \frac{1}{(N/2+4)^2-1} \right) + \dots \right]$$

$$\dots + A_{N-2} \left( \frac{1}{1 \cdot 3} - \frac{1}{(N-2)^2-1} \right) - \left( 1 + \frac{1}{N^2-1} \right) A_N + A_{N+2} \left( \frac{1}{1 \cdot 3} - \frac{1}{(N-2)^2-1} \right) + \dots \Big].$$

If the coefficients  $A_r$  fall off slowly then those near  $A_N$  dominate and  $|I_N - I_{N/2}|$  is of the same order of magnitude as  $|a_N|$ ,  $|a_{N-2}|$  or  $|a_{N-4}|$ . This is illustrated in Table 4. We can therefore use  $|I_N - I_{N/2}|$  as a check that both  $a_N$  and  $a_{N-2}$  are not both accidentally small (or vice versa) as in equation (16).

(See overleaf for Table 4)

Table 4

Values of  $|a_N|$ ,  $|a_{N-2}|$ ,  $|a_{N-4}|$  defined by equation (3), and  $|I_N - I_{N/2}|$  defined by equation (4)

	$N$	$ a_N $	$ a_{N-2} $	$ a_{N-4} $	$ I_N - I_{N/2} $
$\int_0^1 \frac{dx}{1+x^2}$	8	0.645(-5)	0.859(-4)	0.940(-3)	0.589(-4)
	16	0.235(-10)	0.425(-9)	0.655(-8)	0.828(-9)
$\int_0^1 \frac{dx}{1+100x^2}$	8	0.156(-1)	0.963(-2)	0.265(-1)	0.997(-2)
	16	0.440(-3)	0.409(-3)	0.242(-3)	0.310(-3)
	32	0.222(-6)	0.373(-6)	0.491(-6)	0.142(-6)
$\int_0^1 \frac{dx}{1-0.98x^4}$	8	0.252(1)	0.262(1)	0.294(1)	0.960(0)
	16	0.732(0)	0.761(0)	0.853(0)	0.954(-1)
	32	0.744(-1)	0.774(-1)	0.868(-1)	0.318(-2)

## Book Review

*Modern Factor Analysis*, by HENRY H. HARMAN, Second edition, revised, 1967; 474 pages. (Chicago and London: The University of Chicago Press, \$12.50 (104s..))

Factor analysis has been applied in many fields and, it seems, to research problems of all kinds. Among the applications listed in this book, for instance, is the investigation by Sackman and Munson, reported in the *ACM Journal* in 1964 into computer operating time and system capacity for man-machine digital systems. The application of statistical techniques and mathematical models to such problems is gratifying and this kind of applicability may be regarded as a recommendation in itself for the factor approach. It should be pointed out, however, that factor analysis has been generally considered to be a method employing geometrical concepts born out of the necessity to interpret multi-dimensional relationships between variables. This analysis exploits the variations and correlations of the variables, and the rather difficult statistical theory underlying some techniques has not yet been completely worked out. A consequence of this is that significance testing is not always available in applications. In any case, the process of identification of factors has inherent non-uniqueness which causes difficulties of interpretation. Nevertheless, factor analysis with its variety of techniques will continue to provide a valuable means of interpreting data for an increasing number of applied problems.

This book is the second edition of an important text which first appeared eight years ago dealing with the methodology of factor analysis. There has been a considerable revision of the structure and content of many chapters in order to reflect the changed emphasis between the various factor tech-

niques. Principally these changes concern the shift from hand-machine to computer techniques; many flow diagrams and detailed references to computer software are given in the book. Another improvement is the more general use of matrix notation which makes the presentation more consistent.

The first four parts of the book embrace the foundations of factor analysis, direct solutions, derived solutions and factor measurements. A final part of the book consists of problems and solutions. Used as a textbook a student may well find it inconvenient to have not only answers at the end of the book but problems also. An elementary introduction to matrices and Cartesian geometry is included in two chapters of the first part. The numerical processes of factor analysis, the solution of linear equations, matrix inversion, determination of eigenvalues and rotation of axes are discussed in turn in separate parts of the book, and detailed descriptions of hand-machine processes are given. References to more efficient developments in computer methods developed in the past decade are mentioned briefly but not discussed.

This book will clearly continue to serve as a valuable text for research workers who are concerned with the interpretation of multivariate data whose needs are not fulfilled by the more widely used and understood techniques like multiple regression analysis. It still provides the best introduction to the terminology, concepts and methodology of factor analysis. The presentation throughout is of a high standard and the author has taken pains to strengthen the content of this second edition, not least the bibliography in which almost one third of the 550 listed works have appeared since the publication of the first edition.

R. W. HIRNS (Oxford)