



If we denote the computed  $S_{ij}$  by  $\bar{S}_{ij}$  and let  $\epsilon_{ij} = \bar{S}_{ij} - S_{ij}$ , then

$$\bar{S}_{ij} = \bar{S}_{2i,j-1} + \bar{S}_{2i-1,j-1} + r_{ij},$$

where  $r_{ij}$  is the round-off introduced in the step which computes  $\bar{S}_{ij}$ . As before,

$$\epsilon_{ij} = \sum_{\sigma_{ij}} r_{\sigma_{ij}},$$

$$|\epsilon| = |\epsilon_k| \leq \eta \sum_{\sigma_{1k}} 2^{p_{\sigma_{1k}}},$$

where  $\sigma_{ij}$  is the set of all index-pairs of the operations needed to get  $S_{ij}$ , and  $p$  denotes the exponents of the intermediate results. Now, if  $|a_i| < a$ , then clearly

$$\begin{aligned} \bar{S}_{ij} &\leq 2^j a, \\ 2^{p_{ij}} &\leq 2^{j+1} a, \end{aligned}$$

so that

$$|\epsilon| \leq \eta \sum_{\sigma_{1k}} 2^{p_{\sigma_{1k}}} \leq 2\eta a \sum_{j=1}^k \sum_{i=1}^{n/2^j} 2^j = 2\eta a k n,$$

or

$$|\epsilon| \leq 2\eta a l n_2 n. \quad (7)$$

This is better than the error bound (5) by a factor of  $n/(2l n_2 n)$  and we can expect significantly better results from this method.

## Comparison of Several Adaptive Newton-Cotes Quadrature Routines in Evaluating Definite Integrals with Peaked Integrands

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This report compares the performance of five different adaptive quadrature schemes, based on Newton-Cotes ( $2N + 1$ ) point rules ( $N = 1, 2, 3, 4, 5$ ), in approximating the set of definite integrals  $\int_{-1}^1 (x^2 + p^2)^{-1} dx$  with relative accuracy  $\epsilon$ .

**KEY WORDS AND PHRASES:** adaptive Newton-Cotes quadrature, quadrature scheme comparison, definite integral evaluation, adaptive numerical integration, Newton-Cotes integration, peaked integrand integration, quadrature efficiency plot, Newton-Cotes rules applications, Newton-Cotes rules modifications

**CR CATEGORIES:** 5.10, 5.16

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## 4. Numerical Results and Conclusions

As a typical case, we carried out the addition of a sequence of random numbers uniformly distributed in  $(0, 1)$ . The results were computed on the CDC 6600 using a simulated 24-bit addition with truncation, and the comparison was done by calculating the sums via the full 48-bit addition. With twenty trials, each consisting of adding 2048 random numbers, the following results were obtained:

average error for recursive summation = .0419,

average error for improved method = .0003.

The observed errors are comparable to the bounds (5) and (7) which are about  $2^{-2}$  and  $11 \times 2^{-12}$ , respectively. (In this example it is reasonable to expect a better result by taking average values for  $a$  and  $\eta$ ; thus, with  $a = .5$  and  $\eta = \frac{1}{2} \times 2^{-24}$ , the estimates become .0625 and .0006, respectively.)

The method described here has of course some disadvantages: it is more difficult to program than the standard method, and it is difficult to use unless all numbers are available at the start of the summation. However, where these factors are not a problem and where high accuracy is desired, it appears to be superior to recursive summation.

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## Introduction

High degree Newton-Cotes quadrature rules have seldom been used in practice because they occasionally fail to converge or they contain weights of different signs. This report shows, by numerical experiment only, that there are certain quadratures for which the rate of convergence increases with the use of higher degree Newton-Cotes rules, used adaptively, and demonstrates the advantage of adaptive methods over a nonadaptive rule in approximating integrals having peaked integrands.

McKeeman [1-3] and Davis and Rabinowitz [4] describe the use of quadrature rules in an adaptive manner by means of algorithms. Lyness [5] gives a thorough description of the adaptive Simpson rule, together with suggested modifications.

## Quadrature Schemes Used

Five adaptive integration schemes are used. The first (ANC3) is the adaptive Simpson rule incorporating modifications 1, 2, and 3 of [5], and is of overall polynomial degree 5. The others have the same structure but are based on higher degree Newton-Cotes rules and incorporate the appropriate generalization of the same three modifica-

tions. These schemes are referred to as ANC5, ANC7, ANC9, and ANC11, they are based on the 5, 7, 9, and 11 point Newton-Cotes rules, and are of polynomial degree 7, 9, 11, and 13, respectively. In particular, if  $\epsilon$  is the total absolute error allowed and

$$Q_N[a, a+h]f(x) = \sum_{j=1}^{2N+1} a_j f(x_j)$$

is the  $(2N+1)$  Newton-Cotes rule, convergence is achieved over the interval  $[a, a+h]$  if for

$$\Delta = Q_N[a, a+h]f(x) - \left( Q_N\left[a, a+\frac{h}{2}\right]f(x) + Q_N\left[a+\frac{h}{2}, a+h\right]f(x) \right), \quad |\Delta| \leq \frac{(2^{2N+1}-1)\epsilon}{2^r},$$

where

$$h = (B-A)2^{-r}.$$

If this convergence criterion is not satisfied and if  $r < 30$ , the interval is bisected,  $r$  is replaced by  $r+1$ , and, after function evaluations at the new mesh points, the above test is repeated. If the convergence criterion is satisfied or if

$$r = 30, \quad Q_N\left[a, a+\frac{h}{2}\right]f(x) + Q_N\left[a+\frac{h}{2}, a+h\right]f(x) + \Delta/(2^{2N+1}-1)$$

is accepted as an approximation for the integral over  $[a, a+h]$ , this approximation being of degree  $2N+3$ . Finally, these component approximations and error estimates are summed to obtain a final or total approximation over  $[A, B]$ .

In addition, an integration scheme called ROMBERG is used, to put into quantitative perspective the advantage of adaptive techniques for peaked integrands. The ROMBERG scheme is described by Bauer, Rutishauser, and Stiefel in [7].

### Investigations Conducted

Numerical integrations were carried out using the five different adaptive Newton-Cotes rules and the ROMBERG technique in approximating several sets of definite integrals. In each case, an input parameter  $\epsilon$  prescribes the error. A routine is termed the most efficient if its result satisfies the error criterion  $\epsilon$  while requiring the least number of function evaluations. The actual error in each result is usually much smaller than  $\epsilon$ .

The results of one set of numerical integrations are described here and displayed in Figures 1, 2, and in Table I. Information concerning the computations and results of approximating an additional two sets of definite integrals can be obtained from [6].

### Computations

The set of definite integrals  $\int_{-1}^1 (x^2+P^2)^{-1} dx$  has been evaluated with  $P$  ranging from 1 to  $10^{-4}$  and  $\epsilon$  ranging from 1 to  $10^{-8}$ . For small  $P$  the integrand has a peak of height  $P^{-2}$  at the origin, is approximately 1 at the end points, and the value of the integral is approximately equal to  $\pi P^{-1}$ .

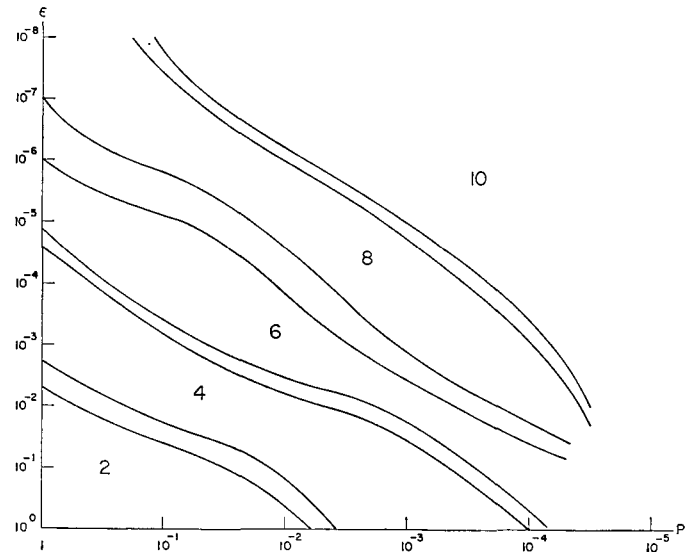


FIG. 1. Results using the adaptive Newton-Cotes rules for the quadrature  $I = \int_{-1}^1 (x^2+P^2)^{-1} dx$

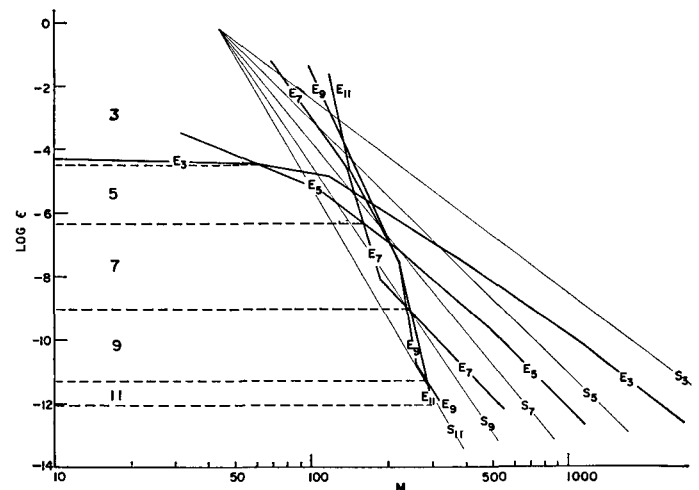


FIG. 2. Error curves of the adaptive Newton-Cotes  $(2N+1)$ -point rules in approximating  $I = \int_{-1}^1 (x^2+P^2)^{-1} dx$ , ( $P=10^{-3}$ ). A point  $(M, \epsilon)$  located in region  $(2N+1)$  indicates that the  $(2N+1)$ -point adaptive Newton-Cotes routine obtained the accuracy  $\epsilon I$  with the least number  $M$  of function evaluations of the routines tested.

TABLE I

<i>Routine</i>	<i>Number of function evaluations</i>	<i>Convergence criterion</i>	<i>Accuracy obtained</i>
$P = 10^{-2}$			
Romberg	1025	$\epsilon = 10^0$	$\epsilon I \simeq 10^{-3}$
ANC3	65		
ANC5	113		
ANC7	145		
ANC9	193		
ANC11	201		
Romberg	4097	$\epsilon = 10^{-1.6}$	$\epsilon I \simeq 10^{-6}$
ANC3	289		
ANC5	129		
ANC7	169		
ANC9	225		
ANC11	241		
Romberg	8193	$\epsilon = 10^{-2.6}$	$\epsilon I \simeq 10^{-8}$
ANC3	601		
ANC5	353		
ANC7	193		
ANC9	257		
ANC11	281		
Romberg	16385	$\epsilon = 10^{-7.6}$	$\epsilon I \simeq 10^{-11}$
ANC3	2305		
ANC5	1073		
ANC7	529		
ANC9	449		
ANC11	321		

 $P = 10^{-3}$ 

Romberg	4097	$\epsilon = 10^0$	$\epsilon I \simeq 10^{-5}$
ANC3	209		
ANC5	193		
ANC7	265		
ANC9	321		
ANC11	401		
Romberg	8193	$\epsilon = 10^{-1.8}$	$\epsilon I \simeq 10^{-8}$
ANC3	993		
ANC5	497		
ANC7	289		
ANC9	353		
ANC11	441		
Romberg	16385	$\epsilon = 10^{-4.8}$	$\epsilon I \simeq 10^{-10}$
ANC3	2441		
ANC5	1009		
ANC7	721		
ANC9	385		
ANC11	481		
Romberg	32769	$\epsilon = 10^{-7.6}$	$\epsilon I \simeq 10^{-12}$
ANC3	6161		
ANC5	2097		
ANC7	1153		
ANC9	865		
ANC11	641		

 $P = 10^{-4}$ 

Romberg	8193	$\epsilon = 10^0$	$\epsilon I \simeq 10^{-6}$
ANC3	617		
ANC5	353		
ANC7	361		
ANC9	449		
ANC11	561		

TABLE I—Continued

<i>Routine</i>	<i>Number of function evaluations</i>	<i>Convergence criterion</i>	<i>Accuracy obtained</i>
Romberg	16385	$\epsilon = 10^{-1.2}$	$\epsilon I \simeq 10^{-8}$
ANC3	3209		
ANC5	673		
ANC7	385		
ANC9	481		
ANC11	601		
Romberg	32679	$\epsilon = 10^{-2.2}$	$\epsilon I \simeq 10^{-10}$
ANC3	6417		
ANC5	1873		
ANC7	913		
ANC9	513		
ANC11	641		
Romberg	65356	$\epsilon = 10^{-5.6}$	$\epsilon I \simeq 10^{-12}$
ANC3	12817		
ANC5	3585		
ANC7	1825		
ANC9	1217		
ANC11	801		

## Results

Results using the adaptive Newton-Cotes rules for the quadrature  $I = \int_{-1}^1 (x^2 + P^2)^{-1} dx$  are displayed in Figure 1 and are to the required accuracy  $\epsilon I$ . If the point  $(P, \epsilon)$  lies in the zone numbered  $2N + 1$ , the adaptive Newton-Cotes  $(2N+1)$ -point rule is the most efficient of those tested.

The actual demarkation lines between zones are not regular. These irregularities are due, in part, to the fact that the number of points used by the adaptive Newton-Cotes rule of degree  $2N + 1$  in approximating an integral over  $(a, a+h)$  is restricted to numbers of the form  $8KN + 1$  ( $K=1, 2, 3, \dots$ ). If the integrand function is altered slightly, the demarkation line is different in detail but has the same general configuration. In Figure 1 the "buffer zones" between distinct zones indicate the general width of these irregularities.

Also, an important feature of the numerical results is the considerable difference in the number of function values required by the various schemes in a particular problem of this type. In order to show this, error curves of the adaptive Newton-Cotes rules for the quadrature  $I$  and a particular value of  $P$  are displayed in Figure 2. The error curves of the adaptive Newton-Cotes  $(2N+1)$ -point rules are labeled  $E(2N+1)$ ; the projections of the intersection points onto the  $\epsilon$ -axis define, for fixed  $P$ , the log  $\epsilon$  interval over which the  $(2N+1)$ -point rule is most efficient, in terms of points  $M$  required; and the lines  $S_3, S_5, S_7, S_9$ , and  $S_{11}$  with slopes 6, 8, 10, 12, and 14, respectively, indicate the rate of convergence of these rules.

Finally, tables comparing the results of approximating

$\int_{-1}^1 (x^2 + P^2)^{-1} dx$ , ( $P = 10^{-2}, 10^{-3}, 10^{-4}$ ) using the ROMBERG technique and the five adaptive schemes are presented (Table I) in order to illustrate the advantage of adaptive techniques over a nonadaptive technique for this type of integrand.

These results are of interest because they indicate that if the integrand has a high, sharp peak, or if great accuracy is required, an adaptive high degree rule is most efficient. This is in contradiction to the more familiar state of affairs in which sharp peaks are associated with inefficient polynomial approximations and the use of low degree rules.

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# Incorporating Origin Shifts into the QR Algorithm for Symmetric Tridiagonal Matrices

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The QR iteration for the eigenvalues of a symmetric tridiagonal matrix can be accelerated by incorporating a sequence of origin shifts. The origin shift may be either subtracted directly from the diagonal elements of the matrix or incorporated by means of an implicit algorithm. Both methods have drawbacks: the direct method can unnecessarily degrade small eigenvalues, while the implicit method can effectively lose the shift and thereby retard the convergence. This paper presents a new method which has neither drawback.

**KEY WORDS AND PHRASES.** eigenvalues, eigenvectors, QR method, origin shifts, symmetric tridiagonal matrix

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This paper gives the theoretical background of Algorithm 384 "Eigenvalues and eigenvectors of a real symmetric matrix," by the same author, which appears on pages 369-371 of this issue.

## 1. Introduction

The QR iteration for the eigenvalues of a matrix  $A$  starts with  $A_0 = A$  and defines a sequence of matrices  $A_i$  by the formulas

$$\begin{aligned} A_i &= Q_i R_i, \\ A_{i+1} &= R_i Q_i, \end{aligned} \quad (1.1)$$

where  $Q_i$  is unitary and  $R_i$  is upper triangular. When  $A$  is real symmetric with distinct eigenvalues,  $A_i$  converges to a diagonal matrix whose nonzero elements are the eigenvalues of  $A$ , and under mild restrictions the eigenvalues appear in descending order of magnitude.

The basic QR algorithm can be modified to include an origin shift  $k_i$ , namely,

$$\begin{aligned} A_i - k_i I &= Q_i R_i, \\ A_{i+1} &= R_i Q_i + k_i I. \end{aligned} \quad (1.2)$$

If  $k_i$  is suitably chosen, the rate of convergence of the element in the lower right-hand corner of  $A_i$  to an eigenvalue of  $A$  is increased remarkably. A discussion of the two most important shifting strategies is found in [5]. This problem will not concern us here. Rather, the object of this paper is to propose a scheme for carrying out (1.2) for symmetric tridiagonal  $A$  when  $k_i$  is given. The scheme avoids on the one hand the dangers of subtracting  $k_i I$  from  $A_i$  directly, thereby overwhelming small diagonal elements of  $A_i$ , and on the other hand the dangers of an indirect scheme in which the effect of a small shift is overwhelmed by a few large elements of  $A_i$ .