Optimal quadrature formulae

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We define a quadrature formula to be optimal if it minimizes the multiplier E in an error bound of the form

$$E\left\{\int_0^1 |x^{(n)}(t)|^p dt\right\}^{1/p}$$

or $$E\{\sup_{0\leqslant t\leqslant 1} |x^{(n)}(t)|\} \text{ (corresponding to } p = \infty)$$

for functions $x(t)$ for which the term in brackets is bounded.

In this paper we study the case $n = 2$ for which we may derive optimal quadrature formulae for all p, and discuss some of their properties. We conclude that the best choice of p is 2 and apply this result to obtain formulae for $n = 4$ and 6, which are shown to be more accurate than formulae used previously.

1. Introduction

The most commonly used methods for approximate evaluation of definite integrals up to the present have been the trapezoid, Simpson and Gaussian rules. Other formulae exist, such as Chebyshev's, but they have been of limited value in practice. For most purposes these methods have been successful, the first two for functions with singularities (in the complex plane) near the range of integration, and the last for functions without this property. That this should be so can be seen from a consideration of the classical error bounds in the three cases. (We take m points in each formula and give the error bound for $\int_0^1 x(t)dt$.)

Trapezoid rule $$\frac{1}{12(m-1)^2}x''(\xi_1) \qquad 0<\xi_1<1$$

Simpson's rule $$\frac{1}{90(m-1)^4}x^{(iv)}(\xi_2) \qquad 0<\xi_2<1$$

Gauss rule $$\frac{(m!)^4}{(2m+1)(2m!)^3}x^{(2m)}(\xi_3) \quad 0<\xi_3<1$$

From these error bounds we see that the trapezoid rule is going to be better than the others if $x''(t)$ is bounded in [0, 1], but $x^{(iv)}(t)$ and higher derivatives are not. Similarly we expect Simpson's rule to be better if $x^{(iv)}(t)$ is bounded and higher derivatives are not. In any case if the "size" of the 2mth derivative increases too rapidly with m, we should use Simpson's rule rather than Gaussian quadrature.

We are therefore led to consider quadrature formulae in which we use information on bounds of some specified derivative, and we may ask what is the best formula to use if our function is of bounded nth derivative. It turns out to be convenient at this stage to generalize our meaning of bounded to *bounded in norm*, and define the L^p norm of a function $x(t)$ by

$$||x||_p = \left\{\int_0^1 |x(t)|^p dt\right\}^{1/p} \qquad 1 \leqslant p < \infty$$

$$||x||_\infty = \sup_{0\leqslant t\leqslant 1} |x(t)|.$$

A function x will be bounded in L^p norm if, for some constant M,

$$||x||_p < M.$$

(When $p = \infty$ this reduces to our ordinary meaning of boundedness.)

Now if we assume our integration formula is to be exact for functions whose $(n-1)th$ derivative vanishes in (0, 1), we know by Peano's theorem (cf. Davis (1963), p. 70) that the error can be expressed in the form

$$\int_0^1 x^{(n)}(t)y(t)dt \tag{1}$$

where $y(t)$ can be shown to be of the form

$$y(t) = \frac{t^n}{n!} - \sum_1^m A_i\frac{(t-t_i)_+^{n-1}}{(n-1)!} \tag{2}$$

where $$(t-t_i)_+^{n-1} = \begin{cases}(t-t_i)^{n-1} & t \geqslant t_i\\ 0 & t < t_i\end{cases}$$

and A_i and t_i are the coefficients and points of the quadrature formula respectively

with $$A_i = y^{(n-1)}(t_i-) - y^{(n-1)}(t_i+).$$

We have a set of subsidiary conditions on the form (2) which can be expressed as

$$\sum_1^m A_i\frac{(t-t_i)^{n-1}}{(n-1)!} \equiv \frac{t^n-(t-1)^n}{n!} \tag{3}$$

leaving $2m - n$ free parameters among the A_i and t_i, and so we must clearly have $2m > n$ for a well posed problem.

From Hölder's inequality we can bound the error (1) by

$$||y(t)||_p||x^{(n)}(t)||_{p'}$$

where $$\frac{1}{p}+\frac{1}{p'} = 1$$

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and we define our formula to be optimal if the first term $||y(t)||$ is minimized with respect to the A_i and t_i. This minimal value depends on three numbers n, m and p. The first, n, which we refer to as the *order* of the formula will always be fixed in advance, and m can be increased to obtain greater accuracy; however, p is to some extent at our disposal. Sard (1949) suggested that one should take $p = 2$ on the grounds of ease of computation. We shall show that for formulae for $n = 2$, which are easily obtained for all p, this choice gives smaller errors for a large range of functions than $p = 1$ or ∞, the two other measures often used. Krylov (1962) derives some formulae of this type by slightly different arguments but gives no comparison of their relative merits. We shall show that for the choice of $p = 2$, we obtain formulae that are "nearly" fourth order, in a sense that will become clear in §7.

2. Optimal quadrature formulae for $y(t)\epsilon L^p$, $1 \leqslant p < \infty$

We are here considering the case $n = 2$, so $y(t)$ is a piecewise quadratic with leading coefficient $\frac{1}{2}$, and continuous at each node t_i. Thus in each interval $[t_i, t_{i+1}]$ we may write

$$2y(t) = y_i(t) = a_i + b_i t + t^2 = (t - \xi_i)(t - \eta_i)$$

where we shall take $\xi_i < \eta_i$, and ξ_i and η_i are in $[t_i, t_{i+1}]$ for an optimal formula (Stern (1966)).

Since we have $2(m - 1)$ independent parameters in this case, and we know $a_0 = b_0 = 0$, $a_m = 1$, $b_m = -2$, we shall use the remaining a_i, b_i as our parameters for minimizing $y(t)$.

We may note here that

$$A_i = \tfrac{1}{2}(b_{i-1} - b_i) = \tfrac{1}{2}(\xi_i + \eta_i - \xi_{i-1} - \eta_{i-1}). \quad (4)$$

Now let us determine the optimal choice of $y(t)$ in the sense of L^p, i.e. the formula which minimizes the error bound, obtained by using Hölder's inequality.

If $E^{1/p}$ is the L^p norm of $2y(t)$, then

$$E = \sum_i \left\{\int_{t_i}^{\xi_i} y_i^p dt + \int_{\xi_i}^{\eta_i} (-y_i)^p dt + \int_{\eta_i}^{t_{i+1}} y_i^p dt\right\}. \quad (5)$$

To minimize E we set

$$\left.\begin{aligned} \frac{\partial E}{\partial a_i} &= 0 \\ \frac{\partial E}{\partial b_i} &= 0 \end{aligned}\right\} \quad i = 1, \ldots, m-1. \quad (6)$$

From the combination

$$\frac{dy_i}{dt} = b_i\frac{\partial E}{\partial a_i} + 2\frac{\partial E}{\partial b_i} = 0 \quad (7)$$

we obtain

$$y_i(t_i) = y_i(t_{i+1}) \quad (8)$$

and since $t_i \neq t_{i+1}$,

$$t_{i+1} + t_i = \eta_i + \xi_i. \quad (9)$$

The first equation of (6) can be transformed using (9) to obtain

$$\int_0^{-\frac{t_i-\xi_i}{\eta_i-\xi_i}} \{S(1 + S)\}^{p-1} dS = \frac{\Gamma(p)^2}{2\Gamma(2p)}. \quad (10)$$

It follows that

$$\frac{t_i - \xi_i}{\eta_i - \xi_i} = -K \quad (11)$$

where K is a function of p but independent of i. A full discussion of the properties of K is given by Stern (1966) §V.5.

Since $y(t)$ is continuous at t_i, we have for $i=2, \ldots, m-1$

$$(t_i - \xi_i)(t_i - \eta_i) = (t_i - \xi_{i-1})(t_i - \eta_{i-1}). \quad (12)$$

From (9), (11) and (12) we obtain

$$2t_i = t_{i+1} + t_{i-1}. \quad (13)$$

So, for any second order optimal quadrature formula, the points at which the function values are taken must be equally spaced.

Since $t_m = 1 - t_1$ by symmetry, we obtain

$$t_i = t_1 + \frac{i-1}{m-1}(1 - 2t_1) \quad (14)$$

$$= t_1 + (i-1)h \quad (15)$$

where h will be referred to as the *step length*.

It now remains to evaluate t_1. We note that $a_0 = b_0 = 0$ and $y(t)$ is continuous at t_1, from which it follows that

$$t_1 = h\frac{\sqrt{[K(1+K)]}}{1+2K}. \quad (16)$$

So writing

$$\lambda = \frac{\sqrt{[K(1+K)]}}{1+2K} \quad (17)$$

we obtain

$$h = \frac{1}{2\lambda + m - 1}. \quad (18)$$

From (4) and (9) we see that

$$A_i = h \qquad i \neq 1, m \quad (19)$$

$$A_1 = A_m = \frac{2\lambda + 1}{2}h. \quad (20)$$

3. Norms of the remainder

We shall next evaluate the following norms of $y(t)$,

$$E_1 = ||y(t)||_1,\ E_2 = ||y(t)||_2,\ E_3 = ||y(t)||_\infty.$$

Let us write

$$\theta = \frac{K}{1+2K}. \quad (21)$$

Then from (9) and (11) we obtain

$$\left.\begin{aligned}\eta_i &= \theta t_i + (1-\theta)t_{i+1}\\ \xi_i &= (1-\theta)t_i + \theta t_{i+1}.\end{aligned}\right\} \tag{22}$$

After some elimination we see that

$$\int_{t_i}^{\xi_i}\{t^2 - (\xi_i + \eta_i)t + \xi_i\eta_i\}dt - \int_{\xi_i}^{\eta_i}\{t^2 - (\xi_i + \eta_i)t + \xi_i\eta_i\}dt + \int_{\eta_i}^{t_{i+1}}\{t^2 - (\xi_i + \eta_i)t + \xi_i\eta_i\}dt$$

$$= \tfrac{1}{6}h^3\{2(1-2\theta)^3 + 6\theta(1-\theta) - 1\} \tag{23}$$

whence

$$E_1 = \tfrac{1}{12}h^2\{2(1-2\theta)^3 + 6\theta(1-\theta) - 1\} + \tfrac{1}{6}h^2t_1(4\theta-1)(2\theta-1)^2. \tag{24}$$

Similarly

$$E_2^2 = \tfrac{1}{120}h^4\{30\theta^2(1-\theta)^2 - 10\theta(1-\theta) + 1\} + \tfrac{1}{60}h^4t_1(2\theta-1)^2(60(1-\theta)-1). \tag{25}$$

Finally to discuss E_3 we observe that $|y(t)|$ takes its supremum in $[t_i, t_{i+1}]$ either at t_i or t_{i+1} or at the point at which its derivative vanishes, i.e. $t^* = \frac{1}{2}(t_i + t_{i+1})$.

$$y(t_i) = y(t_{i+1}) = \tfrac{1}{2}\theta(1-\theta)h^2 \tag{26}$$

$$y(t^*) = \tfrac{1}{8}(1-2\theta)^2h^2 \tag{27}$$

whence

$$E_3 = \begin{cases}\tfrac{1}{2}\theta(1-\theta)h^2 & \tfrac{1}{2}(1-\tfrac{1}{2}\sqrt{2}) < \theta < \tfrac{1}{2}(1+\tfrac{1}{2}\sqrt{2})\\ \tfrac{1}{8}(2\theta-1)^2h^2 & \theta < \tfrac{1}{2}(1-\tfrac{1}{2}\sqrt{2}) \text{ or } \theta > \tfrac{1}{2}(1+\tfrac{1}{2}\sqrt{2}).\end{cases} \tag{28}$$

4. Special formulae

We next derive two important special cases:

(i) $p = 1, p' = \infty$

In this case we find from (10) and (11) that $K = \frac{1}{2}$ and so obtain a formula for which E_1 is a minimum; it will be referred to as *formula* 1. The various norms of $y(t)$ for it are given in **Table 1**.

(ii) $p = p' = 2$

In this case we find from (10) and (11) that $K = \frac{1}{2}(\sqrt{3} - 1)$ and so obtain a formula for which E_2 is a minimum; it will be referred to as *formula* 2. The various norms of $y(t)$ for it are also given in **Table 1**.

5. Optimal quadrature formulae for $y(t)\epsilon L^\infty$

We next derive the formula for which E_3 takes its minimum value which was not covered by the previous work. Since we wish to minimize the supremum of $|y(t)|$, we use Chebyshev's theorem, as extended by Johnson (1960) that $y(t)$ takes its maxima and minima alternately with equal magnitude N^2 and alternating sign. Since $y(t)$ is piecewise quadratic, these extrema must come at the points t_i and once in each sub-range $[t_i, t_{i+1}]$. In each sub-range $y'(t)$ vanishes at the point

$$t^* = \tfrac{1}{2}(\xi_i + \eta_i). \tag{29}$$

We therefore have

$$\left.\begin{aligned}y(t_{i+1}) &= \tfrac{1}{2}(t_{i+1} - \xi_i)(t_{i+1} - \eta_i) = N^2\\ y(t_i) &= \tfrac{1}{2}(t_i - \xi_i)(t_i - \eta_i) = N^2\end{aligned}\right\} \tag{30}$$

$$y(t^*) = \tfrac{1}{8}(\eta_i - \xi_i)^2 = N^2. \tag{31}$$

Table 1.—Data for second order formulae

Formula	λ	$\frac{E_1}{h^2}$	$\frac{E_2}{h^2}$	$\frac{E_3}{h^2}$
Midpoint rule	$\frac{1}{2}$	$\frac{1}{24}$	$\frac{1}{8\sqrt{5}}$	$\frac{1}{8}$
Formula 1	$\frac{\sqrt{3}}{4}$	$\frac{1}{32}$	$\frac{1}{32}\sqrt{\left(\frac{23+2h\sqrt{3}}{15}\right)}$	$\frac{3}{32}$
Formula 2	$\frac{1}{\sqrt{6}}$	$\frac{1}{18\sqrt{3}}\left(1 - \frac{h}{\sqrt{6}}(2-\sqrt{3})\right)$	$\frac{1}{12\sqrt{5}}$	$\frac{1}{12}$
Formula 3	$\frac{1}{2\sqrt{2}}$	$\frac{1}{48}(2\sqrt{2} - 1 - h(2-\sqrt{2}))$	$\frac{1}{16}\sqrt{\left(\frac{7-2h\sqrt{2}}{15}\right)}$	$\frac{1}{16}$
Trapezoid rule	0	$\frac{1}{12}$	$\frac{1}{2\sqrt{30}}$	$\frac{1}{8}$

Table 2.—The μ function

m	μ	p
2	0·3660254038	16
3	0·3843671526	4·8
4	0·3915674722	3·6
5	0·3954260347	3·1
10	0·4022980811	2·4
15	0·4043735690	2·3
20	0·4053754997	2·19
25	0·4059657054	2·15
∞	0·4082482905	2

From (30) and (31) we obtain respectively

$$\left.\begin{aligned}\eta_i - \xi_i &= 2N\sqrt{2}\\ \eta_i + \xi_i &= t_{i+1} + t_i.\end{aligned}\right\} \qquad (32)$$

From equations (32) and (12) we obtain

$$2t_i = t_{i+1} + t_{i-1} \qquad (33)$$

and we see that as before the points are equally spaced.

Furthermore it can easily be shown that

$$N = \tfrac{1}{4}h. \qquad (34)$$

It still remains to determine t_1 which is done as in §2 by observing that $y(t)$ is continuous at t_1, so that

$$t_1 = Nh = \tfrac{1}{4}h \qquad (35)$$

giving a formula of the same form as those obtained for $y(t)\epsilon L^p$, with

$$K = \tfrac{1}{2}(\sqrt{2} - 1)$$
$$\theta = \tfrac{1}{2}(1 - \tfrac{1}{2}\sqrt{2}).$$

This formula, for which E_3 is a minimum, will be referred to as *formula 3*, and the various norms of $y(t)$ for it can be found in Table 1. It can be shown (Stern (1966) §V.5) that it is the limiting case of the L^p-optimal formulae as $p \to \infty$.

6. Error bounds for classical quadrature formulae

It will be seen that the various norms calculated in §3 apply to all quadrature formulae in which the points t_i are equally spaced in some interval contained in [0, 1] and all the coefficients except A_1 and A_m are equal. Two such formulae, which are not optimal, are the trapezoid and midpoint rules. In the trapezoid rule $t_1 = 0$, so that $\theta = 0$; and in midpoint rule $t_1 = \frac{1}{2}h$, so that $\theta = \frac{1}{2}$. We therefore include them in Table 1, giving there the various norms of $y(t)$ appropriate to them for comparison with our formulae.

Other classical quadrature formulae, such as Simpson's rule, can be treated in a similar manner (cf. Stern (1966) §V.6), but the results of §3 are not directly applicable to them, and so are not included in this paper.

7. The fourth order case

The second order quadrature formula optimal for L^p depends on one parameter λ which varies with p. Let us now define μ to be that value of λ for which the optimal formula integrates $x(t) = t^2$ exactly (clearly μ depends on the number of points m). Then μ must satisfy

$$\frac{1}{3} = \frac{2\mu + 1}{2}h\{\mu^2h^2 + (\mu + m - 1)^2h^2\} + h\sum_{i=2}^{m-1}(\mu + i - 1)^2h^2. \qquad (36)$$

This becomes

$$\begin{aligned}2(2\mu + m - 1)^3 = 3(2\mu + 1)\{\mu^2 + (\mu + m - 1)^2\}\\ + 6(m - 2)\mu^2 + 6(m - 2)(m - 1)\mu\\ + (m - 2)(m - 1)(2m - 3)\end{aligned} \qquad (37)$$

which on elimination gives

$$4\mu^3 + 6(m - 1)\mu^2 - (m - 1) = 0. \qquad (38)$$

This equation has three real roots, two of which are negative and one which increases monotonically from $\frac{1}{2}(\sqrt{3} - 1)$ to $1/\sqrt{6}$ as m increases from 2 to infinity. The formula for which $\lambda = \mu$ will be referred to as *formula 4.*

Suppose next that ν is the value of λ for which the optimal formula integrates $x(t) = t^3$ exactly. Then ν satisfies

$$\frac{1}{4} = \frac{2\nu + 1}{2}h\{\nu^3h^3 + (\nu + m - 1)^3h^3\} + h\sum_{i=2}^{m-1}(\nu + i - 1)^3h^3. \qquad (39)$$

This becomes

$$\begin{aligned}(2\nu + m - 1)^4 = 2(2\nu + 1)(\nu^3 + (\nu + m - 1)^3)\\ + 4(m - 2)\nu^3 + 6(m - 2)(m - 1)\nu^2\\ + 2(m - 2)(m - 1)(2m - 3)\nu + (m - 2)^2(m - 1)^2\end{aligned} \qquad (40)$$

which on elimination gives

$$8\nu^4 + 16(m - 1)\nu^3 + 6(m - 1)^2\nu^2 - 2(m - 1)\nu - (m - 1)^2 = 0. \qquad (41)$$

This factorizes into

$$(2\nu + m - 1)(4\nu^3 + 6\nu^2(m - 1) - (m - 1)) = 0. \qquad (42)$$

So we see that $\nu = \mu$, and so formula 4 is in fact fourth order. In **Table 2,** we give values of μ and p for various values of m, and it will be seen that p decreases quite rapidly to 2. (p was obtained by using a table for K as a function of p given by Stern (1966) §V.5.)

8. Numerical comparison of second order formulae

The formulae 1, 2, 3, 4 and the trapezoid and midpoint rules were applied to a wide range of functions and

Table 3

Errors in the evaluation of integrals over [0, 1] using second order formulae

INTEGRAND (INTEGRAL)	m	MIDPOINT RULE	FORMULA 1	FORMULA 2	FORMULA 3	FORMULA 4	TRAPEZOID RULE
$t^3 \log t$ (−0·062500)	5	−0·001620	−0·000734	−0·000400	0·000349	−0·000226	0·005082
	10	−0·000413	−0·000147	−0·000053	0·000148	−0·000030	0·001022
	15	−0·000184	−0·000059	−0·000016	0·000075	−0·000009	0·000424
	20	−0·000104	−0·000032	−0·000007	0·000044	−0·000004	0·000230
	25	−0·000067	−0·000020	−0·000004	0·000029	−0·000002	0·000145
$\frac{e^t}{1+t}$ (1·125386)	5	−0·001128	−0·000422	−0·000161	0·000411	−0·000027	0·003527
	10	−0·000283	−0·000088	−0·000020	0·000124	−0·000003	0·000699
	15	−0·000126	−0·000037	−0·000006	0·000058	−0·000001	0·000289
	20	−0·000071	−0·000020	−0·000002	0·000033	−0·000000	0·000157
	25	−0·000045	−0·000012	−0·000001	0·000022	−0·000000	0·000098
$e^{-(1-2t)^2}$ (0·746824)	5	0·004950	0·000920	−0·000507	−0·003516	−0·001231	−0·015454
	10	0·001229	0·000265	−0·000065	−0·000741	−0·000142	−0·003033
	15	0·000546	0·000124	−0·000020	−0·000310	−0·000041	−0·001252
	20	0·000307	0·000071	−0·000008	−0·000169	−0·000017	−0·000680
	25	0·000196	0·000046	−0·000004	−0·000106	−0·000009	−0·000426
$t^3 - \frac{1}{16}(7t-3)_+^2$ (0·059524)	5	0·001101	0·000536	0·000334	−0·000094	0·000232	−0·001907
	10	0·000257	0·000106	0·000053	−0·000055	0·000041	−0·000453
	15	0·000101	0·000032	0·000008	−0·000041	0·000004	−0·000213
	20	0·000048	0·000009	−0·000004	−0·000031	−0·000006	−0·000122
	25	0·000030	0·000005	−0·000003	−0·000020	−0·000004	−0·000076
$(t-e^{-1})_+^2 - (t-2e^{-1})_+^2$ (0·078043)	5	−0·001256	−0·000357	−0·000033	0·000662	0·000132	0·003993
	10	−0·000276	−0·000046	0·000034	0·000197	0·000052	0·000789
	15	−0·000135	−0·000033	0·000002	0·000073	0·000007	0·000313
	20	−0·000080	−0·000023	−0·000004	0·000036	−0·000002	0·000170
	25	−0·000049	−0·000012	0·000000	0·000025	0·000001	0·000106

the errors obtained are to be found in **Table 3**. As will be seen the functions are of a diverse nature, and as expected, formulae 2 and 4 do much better than formulae 1 and 3, which in turn do better than the classical formulae. For further results for other functions, cf. Stern (1966). The difference in error between formula 2 and formula 4 is not on the whole as marked as to justify the extra work involved in the calculation of μ for each m, and so it would appear that the L^2 optimal formula is the best to use in practice. This would agree with Sard's hypothesis (1949) that it is best to use the norm L^2 in the derivation of optimal quadrature formulae. We therefore shall use this hypothesis to derive formulae for larger values of n in §9–10.

9. Fourth order formulae

From symmetry considerations we see that if t_i is a point of the formula so is $1 - t_i$ and both have the same weight A_i. Clearly if $m = 2l + 1$, $t_{l+1} = \frac{1}{2}$. Taking this into account we derive from (2), for $n = 4$,

$$24y(t) = \begin{cases} t^4 - 4 \sum_{i=1}^{l} A_i(t - t_i)_+^3 & 0 \leqslant t \leqslant \frac{1}{2} \\ t^4 - 4 \sum_{i=1}^{l} A_i(1 - t_i - t)_+. & \frac{1}{2} \leqslant t \leqslant 1 \end{cases} \tag{43}$$

The condition (4) reduces in both the cases $m = 2l$ and $m = 2l + 1$ to

$$\sum_{i=1}^{l} A_i(\tfrac{1}{2} - t_i)^2 = \tfrac{1}{24} \tag{44}$$

with, in addition, when $m = 2l$,

$$\sum_{i=1}^{l} A_i = \tfrac{1}{2}. \tag{45}$$

Putting $E = ||y(t)||$ we find on integration that

Table 4

Points and weights for optimal fourth order formula for integrals over [0, 1]

m	t_i	A_i	E
2	0·211325 0·788675	0·500000 0·500000	$3\cdot22227_{10^{-4}}$
3	0·117602 0·500000 0·882398	0·284943 0·430114 0·284943	$3\cdot26121_{10^{-5}}$
4	0·081930 0·347858 0·652142 0·918070	0·198457 0·301543 0·301543 0·198457	$7\cdot68740_{10^{-6}}$
5	0·064593 0·271163 0·500000 0·728837 0·935407	0·156061 0·230694 0·226490 0·230694 0·156061	$2\cdot69578_{10^{-6}}$
6	0·055879 0·229740 0·411764 0·588236 0·770260 0·944121	0·134368 0·188748 0·176884 0·176884 0·188748 0·134368	$1\cdot27467_{10^{-6}}$

$$\tfrac{1}{2}\{24E\}^2 =$$

$$\frac{1}{4608} - \frac{1}{280}\sum_{i=1}^{l} A_i s_i^4\{35 - 56s_i + 56s_i^2 - 32s_i^3 + 8s_i^4\}$$

$$+ \frac{16}{7}\sum_{i=1}^{l} A_i^2 s_i^7 + \frac{8}{35}\sum_{\substack{j=1\\ i>j}}^{l-1} A_i A_j s_i^4\{35s_j^3 - 21s_j^2 s_i + 7s_j s_i^2 - s_i^3\} \tag{46}$$

where

$$s_i = \tfrac{1}{2} - t_i. \tag{47}$$

This function was minimized for $m = 3, 4, 5, 6$ subject to the conditions (9) and (10) using Powell's method (1964), and the resulting points and weights of the optimal quadrature formulae will be found in **Table 4**. The formulae so obtained were then applied, together with other fourth order formulae to a wide range of functions, and the error in the integral was calculated in each case, the results being given in **Table 5**. It will be seen from the table that these optimal formulae do give much smaller errors for any given number of points, m, than any other formula used. (In this table the four point and six point Gaussian formulae used are two point Gauss quadrature applied to two and three sub-intervals respectively. Similarly the six point Chebyshev formula is merely the Chebyshev three point formula applied to half intervals. This was done in order to obtain fourth order formulae for comparison purposes. The formulae due to Sard are given by Meyers and Sard (1950).)

Table 6

Points and weights for optimal sixth order formulae for integrals over [0, 1]

m	t_i	A_i	E
3	0·112702 0·500000 0·887298	0·277778 0·444444 0·277778	$7\cdot41061_{10^{-7}}$
4	0·071333 0·332634 0·667366 0·928667	0·177605 0·322395 0·322395 0·177605	$4\cdot85666_{10^{-8}}$
5	0·052451 0·244680 0·500000 0·755320 0·947549	0·130578 0·237955 0·262934 0·237955 0·130578	$7\cdot73495_{10^{-9}}$
6	0·049564 0·227731 0·430555 0·569445 0·772269 0·950436	0·123081 0·214647 0·162272 0·162272 0·214647 0·123081	$4\cdot96865_{10^{-9}}$

10. Sixth order formulae

By similar reasoning to the fourth order problem we can show for sixth order formulae that $y(t)$ is given by

$$720y(t) = \begin{cases} t^6 - 6\sum_{i=1}^{l} A_i(t - t_i)_+^5 & 0 \leqslant t \leqslant \tfrac{1}{2} \\ (t-1)^6 - 6\sum_{i=1}^{l} A_i(1 - t - t_i)_+^5 & \tfrac{1}{2} \leqslant t \leqslant 1. \end{cases} \tag{48}$$

Condition (3) reduces for $m = 2l$ and $m = 2l + 1$ to

$$\left.\begin{aligned} \sum_{i=1}^{l} A_i s_i^2 &= \frac{1}{24} \\ \text{and} \qquad \sum_{i=1}^{l} A_i s_i^4 &= \frac{1}{160} \end{aligned}\right\} \tag{49}$$

with, when $m = 2l$, in addition

$$\sum_{i=1}^{l} A_i = \tfrac{1}{2}. \tag{50}$$

Table 5

Errors in the evaluation of integrals over [0, 1] using fourth order formulae

m	FORMULA	INTEGRAND $t^5 \log t$	$t^{7/2}$	e^t	$e^{-(1-2t)^2}$	$t^5 - \frac{1}{16}(3t-1)_+^4$	$\frac{e^t}{1+t}$
3	Sard	0·013337	0·003370	0·000581	−0·042470	−0·015104	0·000570
	Chebyshev	−0·003399	−0·000852	−0·000147	−0·009137	0·003230	−0·000148
	Optimal	−0·000624	−0·000145	−0·000023	0·000804	−0·000237	−0·000030
4	Sard	0·006059	0·001519	0·000258	0·016275	−0·005845	0·000263
	Gauss	−0·000635	−0·000166	−0·000061	−0·000241	0·000120	−0·000036
	Optimal	−0·000115	−0·000027	−0·000004	0·000203	−0·000021	−0·000006
5	Sard	0·000617	0·000144	0·000020	−0·000812	0·000201	0·000029
	Optimal	−0·000040	−0·000010	−0·000001	0·000075	0·000015	−0·000002
6	Sard	0·000314	0·000073	0·000011	−0·000544	0·000104	0·000016
	Chebyshev	−0·000241	−0·000058	−0·000006	−0·000093	0·000070	−0·000009
	Gauss	−0·000130	−0·000031	−0·000002	−0·000062	0·000060	−0·000004
	Optimal	−0·000023	−0·000006	−0·000001	0·000043	−0·000001	−0·000001
	Integral	−0·027778	0·222222	0·718282	0·746824	0·033333	1·125386

Table 7

Errors in the evaluation of integrals over [0, 1] using sixth order formulae

m	FORMULA	INTEGRAND $t^7 \log t$	$t^{11/2}$	e^t	$e^{-(1-2t)^2}$	$t^7 - \frac{1}{729}(5t-2)_+^6$	$\frac{e^t}{1+t}$
4	Lobatto	0·0015569	0·0001562	0·0000010	−0·0032352	−0·0062085	0·0000129
	Optimal	−0·0000516	−0·0000053	−0·0000001	−0·0000581	0·0000332	−0·0000007
5	Sard	0·0012192	0·0001227	0·0000026	−0·0024507	−0·0047733	0·0000113
	Chebyshev	−0·0004419	−0·0000441	−0·0000002	0·0008401	0·0016829	−0·0000037
	Optimal	−0·0000065	−0·0000006	0·0000000	−0·0000111	0·0000168	−0·0000001
6	Sard	0·0006898	0·0000691	0·0000004	−0·0013039	−0·0026251	0·0000059
	Gauss	−0·0000203	−0·0000021	−0·0000000	−0·0000095	0·0000406	−0·0000003
	Optimal	−0·0000050	−0·0000005	−0·0000000	−0·0000084	0·0000117	−0·0000001
	Integral	−0·0156250	0·1538462	1·1782818	0·7468241	0·0392857	1·1253861

Putting $E = ||y(t)||$ we find on integration

$$\tfrac{1}{2}\{720E\}^2 = \frac{1}{106496} - \frac{1}{7392}\sum_{i=1}^{l} A_i s_i^6\{231 - 396s_i + 495s_i^2 - 440s_i^3 + 264s_i^4 - 96s_i^5 + 16s_i^6\} + \frac{36}{11}\sum_{i=1}^{l} A_i^2 s_i^{11} + \frac{2}{77}\sum_{\substack{j=1\\ i>j}}^{l-1} A_i A_j s_i^6\{462s_j^5 - 330s_j^4 s_i + 165s_j^3 s_i^2 - 55s_j^2 s_i^3 + 11s_j s_i^4 - s_i^5\}. \quad (51)$$

This was minimized subject to (45) and (46) using Powell's method (1964) and the resulting points and weights will be found in **Table 6** for $m = 3, 4, 5, 6$. These formulae were then applied, together with other sixth order formulae to a wide range of functions, and the errors in the calculation are given in **Table 7**. As in the fourth order case we see that optimal formulae do give much more accurate results than any of the classical quadrature formulae. (The six point Gaussian formula used was that obtained by applying Gauss three point formula to half intervals in order to obtain sixth order formula. The formulae termed Sard's are also the Newton Cotes formulae in the cases here considered.)

11. Conclusion

We have shown a method for finding quadrature formulae that are optimal in the sense that they give much lower errors for functions of a specific class (bounded nth derivative). The method also provides an error bound for such formulae in terms of a bound on the nth derivative. Here we have only discussed the cases $n = 2, 4, 6$, since higher derivatives of the integrand are usually not convenient to handle. However, the same methods can be applied in principle to obtain optimal formulae for any value of n. The amount of computation required increases rapidly with increasing n and m, and such difficulties are discussed by Stern (1966), where a few formulae for $n = 8$ and 10 are given.

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Correspondence

To the Editor,
The Computer Journal.

Sir,

I was interested to read the paper by B. J. Allen on "An investigation into direct numerical methods for solving some calculus of variation problems", which appeared in this *Journal* in August, 1966.

However, once one accepts that the integral must be evaluated numerically it is surely better to use the Ritz method combined with a hill-climbing technique that does not require the evaluation of derivatives. This approach has been used for partial differential equations by Rosenbrock and Storey (*Computational Techniques for Chemical Engineers*, Pergamon, 1966, p. 115).

I am investigating some boundary value problems for ordinary differential equations that arise in chemical engineering by turning the problem into a variational one and using this technique, and have obtained some useful results which I hope to publish shortly.

Yours faithfully,

H. W. PAKES

University of Technology,
Loughborough,
Leics.
8 September 1966.