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Quadrature Rules for Singular Integrals with Application to Schwarz–Christoffel Mappings

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Numerical quadrature rules for singular integrals are presented and error bounds are derived. The rules are simple modifications of composite Newton–Cotes formulas. For singularities of type x^α, $\alpha > -1$, the lowest order rule (modified midpoint rule) has error terms of order Δ^2, $\Delta^{2+\alpha}$, and $\Delta^2 \log(1/\Delta)$, where Δ is the subinterval length. The rule proposed by Davis for integration of the Schwarz–Christoffel equation for conformal mapping of polygons is shown to have error terms of the same order. For polygons with sharp corners, i.e., α close to -1, the number of integration subintervals required for the Schwarz–Christoffel equation can be reduced by several orders of magnitude by use of higher order rules given here. Explicit formulas are given for four rules of most likely utility; they are extensions of the midpoint, trapezoidal, Simpson's, and 4-point rules. © 1988 Academic Press, Inc

I. INTRODUCTION

We shall develop modifications of composite Newton–Cotes quadrature rules applicable to

$$\int_a^b s(x)\, f(x)\, dx, \tag{1.1}$$

where $f(x)$ is "smooth" and $s(x)$ is integrable, but where $s(x)$ or some of its low-order derivatives may be singular.

The rules can be utilized for an arbitrary integrand $F(x)$ by setting

$$\int_a^b F(x)\, dx = \int_a^b s(x)[F(x)/s(x)]\, dx,$$

where $s(x)$ includes the singular character of $F(x)$ and $F(x)/s(x)$ is nonsingular. To

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apply an $(n+1)$-point rule, as defined below, the indefinite integral of $x^m s(x)$, $0 \leqq m \leqq n$ must be available, preferably in analytic form. Typical singular functions to which the method applies are x^α, $\log x$, and, more generally, $x^\alpha(\log x)^p$, $p =$ integer. The method may also be useful when $s(x)$ is nonsingular, but has derivatives much larger than $f(x)$. It may be considered an extension of Filon's method [1, 2] for integrals proportional to $\sin kx$, $k \gg 1$.

This study is motivated by interest in numerical conformal mappings of polygons and regions with corners, where integration of the Schwarz–Christoffel equation or its variants is sought. If the boundary of the region to be mapped has a corner with interior angle ϕ, the method calls for integration of a function with singularity of type x^α, $\alpha = -1 + \phi/\pi$. The singularity is most severe for a "sharp" corner, i.e., for ϕ close to zero and α close to -1.

To integrate over corners, Davis [3] introduced quadrature rule for integrals of type $\Pi(x-d_k)^{\alpha_k}$. The integration interval was divided into subintervals of common length Δ, and on each subinterval, each factor $(x-d_k)^{\alpha_k}$ was replaced by its average.

Young [4] has given singular quadrature prescriptions in terms of matrices for "endpoint" and "midpoint" formulas. Our point of departure is similar and the data in our Section III.A can be made to correspond with his midpoint matrices. Our rules are obtained more simply, however, with a rather small amount of elementary algebra, and we go further; in particular, we analyze and compare convergence rates for composite rules. Atkinson [5] found similar rules but weaker error bounds. His Simpson's rule analog had errors of order Δ^3 for $s(x) = x^\alpha$, while we get $\Delta^{4+\alpha}$ and Δ^4.

The rules in III.A are directly transcribable to a computer program. This is also true of the Gauss–Jacobi approach if a routine for generating the Gauss nodes and weights is available (the Los Alamos routine QUAD was used for the data comparison if IV.B). Sloan and Smith [6] have developed an alternative approach, also of potentially high accuracy, but also requiring supporting subroutines. Still further alternatives are noted in [2] and in Davis and Rabinowitz [7].

In the next section we develop the singular quadrature rules and error bounds. The errors of these rules are compared to Newton–Cotes errors. Section III enumerates the lower order rules—comparable to the midpoint, trapezoidal, Simpson's, and 4-point rules—which we believe are most likely to have practical utility. The modified midpoint rule is the most straightforward to apply and leads directly to Davis's method. In contrast to Davis's experience, however, we show that for x^α-type singularities with α negative, error terms of order $\Delta^{2+\alpha}$ and $\Delta^2 \log(\Delta^{-1})$ may be present. In Schwarz–Christoffel problems with sharp corners and alphas close to -1, the linear dependence of error on Δ may make this approach ineffective. In this case, one may pass to the modified trapezoidal rule, with only a slight complication of arithmetic; this would eliminate errors of order $\Delta^{2+\alpha}$. More generally, it may be expedient to go on to the modified Simpson's rule whose error is of order $\Delta^{4+\alpha}$, or modified 4-point rule, whose leading error is of order $\Delta^4 \log \Delta$ or $(1+\alpha)^{-1} \Delta^4$, for $\alpha < 0$.

Trefethen [8] noted that Gauss–Jacobi quadrature can provide high-precision integration for Schwarz–Christoffel problems. However, application of a simple third- or fourth-order method remains attractive because of its programming simplicity, if it can provide sufficient precision for the needs of the problem at low computer cost.

The last section displays some numerical experiments with these rules.

II. Formulation

A. *Modified Newton Cotes Quadrature Rules*

By suitable subdivision of $[a, b]$ and rescaling, the integral (1.1) can be represented as a sum over terms of the form

$$I=\int_0^1 s(x)\, f(x)\, dx, \tag{2.1}$$

in which the only singularity of $s(x)$ is at $x=0$. Discussion in this section will refer to this standard form.

Divide $[0, 1]$ into N subintervals of length Δ; $N\Delta=1$. Let $x_i=i\Delta$ denote the initial point of the ith interval. I separates into

$$I=\sum_{i=0}^{N-1} I_i, \qquad I_i=\int_{x_i}^{x_{i+1}} s(x)\, f(x)\, dx. \tag{2.2}$$

Then $I_i=I_i^{(0)}+E_i$, where $I_i^{(0)}$ is the approximation to be described and E_i is its error. We write

$$I^{(0)}=\sum_{i=0}^{N-1} I_i^{(0)}, \qquad E=\sum_{i=0}^{N-1} E_i, \qquad I=I^{(0)}+E, \tag{2.3}$$

where $I^{(0)}$ denotes the approximation to I and E is the total error.

We follow the Newton–Cotes methodology used by, e.g., Isaacson and Keller [9] for the initial analysis. For a closed $(n+1)$-point rule for I_i, $[x_i, x_{i+1}]$ is divided into n equal subintervals separated by nodal points $\{y_k\}$, $y_k=x_i+k\,\Delta/n$, $0\leq k\leq n$. For an open $(n+1)$-point rule, the division is into $n+2$ subintervals with $y_k=x_i+(k+1)\,\Delta/(n+2)$. (For better or worse, we retain the convention that an even rule ("$n=$even") has an even number of subintervals, and an odd number of nodes).

Assume $f(x)\in C^{n+2}[0, 1]$ if n is even and $f(x)\in C^{n+1}[0, 1]$ if n is odd. Let M_n be an upper bound for $|f^{(n)}(x)|$ on $[0, 1]$, when it exists.

We now formulate the rule on interval $[x_i, x_{i+1}]$. Let $P_n(x)$ be the nth degree polynomial which agrees with $f(x)$ on the nodes y_k of $[x_i, x_{i+1}]$. Then

$$f(x)=P_n(x)+w_n(x)\, f[y_0, ..., y_n, x],$$

where $f[y_0, ..., y_n, x]$ is the $(n+1)$th-order divided difference and

$$w_n(x) = \prod_{k=0}^{n} (x - y_k).$$

The explicit formula for $P_n(x)$ is

$$P_n(x) = \sum_{k=0}^{n} f(y_k) \frac{w_n(x)}{(x - y_k)\, w_n'(y_k)}, \tag{2.4}$$

where $w_n'(y_k) = [dw_n(x)/dx]_{x=y_k}$. We note a general property of divided differences:

$$(d/dx)^m f[y_0, ..., y_n, x] = m!\, f^{(n+m+1)}(\xi_i)/(n+m+1)!,$$

where ξ_i is in the interval spanned by the y's and x, i.e., ξ_i is in (x_i, x_{i+1}), provided $f(x)$ has the requisite differentiability.

The singular quadrature rule for I_i is

$$I_i^{(0)} = \int_{x_i}^{x_{i+1}} s(x)\, P_n(x)\, dx. \tag{2.5}$$

In Section III, these data are written out for the more practical cases.

The error on the ith interval is

$$E_i = \int_{x_i}^{x_{i+1}} s(x)\, f[y_0, ..., y_n, x]\, w_n(x)\, dx.$$

B. *Bounds on the Errors E_i*

(1) To estimate error bounds, we treat the zeroth interval $[0, \Delta]$, where $s(x)$ has its singularity, as a separate case. We have

$$|E_0| \leqq \int_0^{\Delta} |s(x)\, f[y_0, ..., y_n, x]\, w_n(x)|\, dx \leqq \frac{M_{n+1}}{(n+1)!} e_n,$$

where

$$e_n = \int_0^{\Delta} |s(x)\, w_n(x)|\, dx. \tag{2.6}$$

In turn, $|w_n(x)| \leqq \Delta^{n+1}$ for $0 \leqq x \leqq \Delta$, so that

$$e_n \leqq \Delta^{n+1} \int_0^{\Delta} |s(x)|\, dx. \tag{2.7}$$

(2) To estimate E_i for $i \geqq 1$, first suppose n is even. Define

$$\Omega(x) = \pm \int_{x_i}^{x} w_n(x')\,dx'.$$

where the plus is for a closed rule and the minus for an open rule. We have [9, Chap. 7] $\Omega(x_i) = \Omega(x_{i+1}) = 0$ and $\Omega(x) \geqq 0$ for $x \geqq x_i$, for both types of rules. This permits, after an integration by parts, application of the integral mean value theorem:

$$\begin{aligned} E_i &= \pm \int_{x_i}^{x_{i+1}} s(x) f[y_0, ..., y_n, x]\, d\Omega(x) \\ &= \mp \int_{x_i}^{x_{i+1}} \frac{d}{dx} \{s(x) f[y_0, ..., y_n, x]\}\, \Omega(x)\, dx \\ &= \mp \frac{d}{dx} \{s(x) f[y_0, ..., y_n, x]\}_{x=\xi_i} \int_{x_i}^{x_{i+1}} \Omega(x)\, dx, \\ & x_i \leqq \xi_i \leqq x_{i+1}. \end{aligned}$$

Then

$$|E_i| \leqq \Delta^{n+3} W_n \left[|s'(\xi_i)| \frac{M_{n+1}}{(n+1)!} + |s(\xi_i)| \frac{M_{n+2}}{(n+2)!} \right],$$

where

$$W_n = \Delta^{-n-3} \int_{x_i}^{x_{i+1}} \Omega(x)\, dx = \mp \Delta^{-n-3} \int_{x_i}^{x_{i+1}} x w_n(x)\, dx.$$

Note that W_n is positive, and independent of i and of Δ. Also, put

$$S_0(\Delta) = \sum_{i=1}^{N-1} |s(\xi_i)|, \qquad S_1(\Delta) = \sum_{i=1}^{N-1} |s'(\xi_i)|.$$

Then

$$\begin{aligned} |E| &\leqq \sum_{i=0}^{N-1} |E_i| \\ &\leqq \frac{M_{n+1}}{(n+1)!} \{e_n + \Delta^{n+3} W_n S_1(\Delta)\} + \frac{M_{n+2}}{(n+2)!} \Delta^{n+3} W_n S_0(\Delta). \end{aligned} \tag{2.8a}$$

(3) Next, consider $n =$ odd. We examine only closed rules here, so that $y_n = x_{i+1}$. Analogous bounds could be obtained for odd n and open rules with somewhat more effort, but the additional formulas so obtained do not seem to us of any additional utility. Set

$$\Phi(x)=\int_{x_i}^{x}(x'-y_n)^{-1}\,w_n(x')\,dx'.$$

Then $\Phi(x)\geqq 0$ for $x\geqq x_i$ and the product $(x-y_n)\,\Phi(x)$ vanishes at $x=x_i$ and $x=x_{i+1}$. Therefore, proceeding in analogy to the case of even n,

$$\begin{aligned}E_i&=\int_{x_i}^{x_{i+1}} s(x)\,f[y_0,\ldots,y_n,x](x-y_n)\,d\Phi(x)\\&=\int_{x_i}^{x_{i+1}}\frac{d}{dx}\{s(x)\,f[y_0,\ldots,y_n,x](y_n-x)\}\,\Phi(x)\,dx\\&=\frac{d}{dx}\{s(x)\,f[y_0,\ldots,y_n,x](y_n-x)\}_{x=\xi_i}\\&\quad\times\int_{x_i}^{x_{i+1}}\Phi(x)\,dx,\qquad x_i\leqq\xi_i\leqq x_{i+1},\end{aligned}$$

where the integral mean value theorem was used. We see that

$$|f[y_0,\ldots,y_n,x](y_n-x)\leqq \Delta M_{n+1}/(n+1)!$$

and

$$\begin{aligned}&|(d/dx)\{f[y_0,\ldots,y_n,x](y_n-x)\}|\\&\quad=|(d/dx)\{f[y_0,\ldots,y_{n-1},y_n]-f[y_0,\ldots,y_{n-1},x]\}|\\&\quad\leqq M_{n+1}/(n+1)!.\end{aligned}$$

Hence,

$$|E_i|\leqq\frac{M_{n+1}}{(n+1)!}\,\Delta^{n+2}\,W_n[\Delta|s'(\xi_i)|+|s(\xi_i)|],$$

where

$$W_n=\Delta^{-n-2}\int_{x_i}^{x_{i+1}}\Phi(x)\,d(x-y_n)=-\Delta^{-n-2}\int_{x_i}^{x_{i+1}}w_n(x)\,dx.$$

Again, W_n is positive and independent of i and of Δ. For odd n, the bound on E appears as

$$|E|\leqq\frac{M_{n+1}}{(n+1)!}\,\{e_n+\Delta^{n+3}\,W_nS_1(\Delta)+\Delta^{n+2}\,W_nS_0(\Delta)\}. \qquad (2.8\text{b})$$

C. *Error Comparisons for the Singular Quadrature Rules and Comparison With Newton–Cotes*

For Newton–Cotes, it is generally true that as the number N of subintervals increases and their length $\Delta = N^{-1} \to 0$, the error goes like Δ^{n+2} for even n and like Δ^{n+1} for odd n. On this basis, it is sometimes stated that the even rules are "more efficient." The error variation with Δ for the proposed singular quadrature rules resembles the Newton–Cotes behavior, but with some deviations depending on the singular function.

The bounds on $S_1(\Delta)$ and $S_0(\Delta)$ needed for bounds on the errors of the singular rules may be sought in terms of integrals over $|s'(x)|$ and $|s(x)|$. We explore this through a series of examples.

(1) Let $s(x)$ and $s'(x)$ be bounded by s_M and s'_M on $[0, 1]$. Then e_n, Eq. (2.7), goes like Δ^{n+2} and $S_0(\Delta)$, $S_1(\Delta)$ are bounded by $s_M \Delta^{-1}$ and $s'_M \Delta^{-1}$ as $\Delta \to 0$. The error bounds, Eqs. (2.8a) and (2.8b) show that E decreases like Δ^{n+2} for n even and Δ^{n+1} for n odd. Thus, the Newton–Cotes rate of convergence is reproduced (with somewhat different numerical coefficients), even if higher derivatives of $s(x)$ do not exist.

(2) Let $s(x) = \log(x)$. Then $|s(x)|$ and $|s'(x)|$ are monotonic decreasing. We have

$$|s(\xi_i)| \leqq \Delta^{-1} \int_{x_{i-1}}^{x_i} |s(t)|\, dt, \qquad 1 \leqq i \leqq N,$$

and hence

$$S_0(\Delta) \leqq \Delta^{-1} \int_0^1 |s(t)|\, dt. \tag{2.9}$$

Now, $|s'(t)|$ is not integrable at $t = 0$, but we can put

$$S_1(\Delta) \leqq |s'(\Delta)| + \sum_{i=2}^{N-1} |s'(\xi_i)| \leqq |s'(\Delta)| + \Delta^{-1} \int_\Delta^1 |s'(t)|\, dt. \tag{2.10}$$

For the present case,

$$S_0(\Delta) \leqq \Delta^{-1}, \qquad S_1(\Delta) \leqq \Delta^{-1} + \Delta^{-1} \log(\Delta^{-1}),$$

and also, $e_n \leqq \Delta^{n+2}[\log(\Delta^{-1}) + 1]$.

The leading terms in E go like $\Delta^{n+2} \log(\Delta^{-1})$ for n even and Δ^{n+1} for n odd. This resembles the Newton–Cotes rate of convergence, but is slowed by the factor $\log(\Delta^{-1})$ for even rules.

(3) Let $s(x) = x^\alpha$, $\alpha > 0$. Then $s(x)$ is monotonic increasing and

$$S_0(\Delta) \leqq \sum_{i=1}^{N-2} |s(\xi_i)| + |s(1)| \leqq \Delta^{-1} \int_0^1 |s(t)|\, dt + |s(1)|. \tag{2.11}$$

And regardless of whether $s'(x)$ is increasing or decreasing,

$$S_1(\Delta) \leqq \Delta^{-1} \int_0^1 |s'(t)|\, dt + |s'(1)|.$$

Therefore,

$$S_0(\Delta) \leqq \Delta^{-1} + 1, \qquad S_1(\Delta) \leqq \Delta^{-1} + \alpha.$$

Also, $e_n \to 0$ faster than Δ^{n+2}. Again, the Newton–Cotes rate of convergence in Δ is reproduced.

(4) Let $s(x) = x^\alpha$, $-1 < \alpha < 0$. Then both $|s(x)|$ and $|s'(x)|$ are monotonic decreasing. Instead of (2.9), we use a bound for S_0 which is not singular as $\alpha \to -1$:

$$S_0(\Delta) \leqq |s(\Delta)| + \Delta^{-1} \int_\Delta^1 |s(t)|\, dt \leqq \Delta^\alpha + \Delta^{-1} L_\alpha(\Delta), \tag{2.12}$$

where

$$L_\alpha(\Delta = (1+\alpha)^{-1} (1 - \Delta^{1+\alpha}). \tag{2.13}$$

Proceeding from (2.10), we have

$$S_1(\Delta) \leqq (1-\alpha)\, \Delta^{-1+\alpha} - \Delta^{-1} \leqq 2\Delta^{-1+\alpha}.$$

To appreciate how $L_\alpha(\Delta)$ varies with Δ when α is "close" to -1, define a critical subinterval width Δ_c by

$$\log(1/\Delta_c) = (1+\alpha)^{-1}, \qquad \Delta_c = \exp[-(1+\alpha)^{-1}].$$

Then $L_\alpha(\Delta)$ is approximated by $(1+\alpha)^{-1}$ for the range $0 < \Delta \leqq \Delta_c$, and by $\log(\Delta^{-1})$ for $\Delta_c \leqq \Delta < 1$. Referring to the conformal mapping of a polygon to a line, as an example, suppose the polygon has an interior angle of $\phi = \pi/6$. The Schwarz–Christoffel integral will have a singularity of type x^α, $\alpha = -1 + \phi/\pi = -5/6$, corresponding to $\Delta_c = 2.5 \times 10^{-3}$. Then $L_\alpha(\Delta)$ will vary with Δ like $\log(\Delta^{-1})$ so long as the number of integration subintervals is of the order of 1000 per unit interval, or less.

For this type of singularity, and n even, the dominant terms in the singular quadrature error derive from e_n and S_1 and go like $\Delta^{n+2+\alpha}$. This is inferior to the Newton–Cotes rate of Δ^{n+2}, especially if α is close to -1. For n odd, the dominant term in the error, deriving from S_0, goes like $\Delta^{n+1} L_\alpha(\Delta)$, which is more comparable to the Newton–Cotes rate of Δ^{n+1}. The even n cases are not, in general, "more efficient" than the odd cases. For the mid-point rule ($n = 0$), the dominant error term goes like $\Delta^{2+\alpha}$, while for the trapezoidal rule ($n = 1$), it goes like $\Delta^2 L_\alpha(\Delta)$.

When, however, $f(x)$ is even about the singular point, the $\Delta^{n+2+\alpha}$ error terms for even n are absent. To see this, set (with n even)

$$f(x) = \sum_{k=0}^{n} x^k f^{(k)}(0)/k! + x^{n+1} f^{(n+1)}(0)/(n+1)! + R(x). \tag{2.14}$$

The $n+1$ terms of the sum are treated exactly by an $(n+1)$-point rule. There will be $\Delta^{n+2+\alpha}$ error terms proportional to $f^{(n+1)}(0)$, but for n even and $f(x)$ even about $x=0$, $f^{(n+1)}(0)=0$. Also, there are no $\Delta^{n+2+\alpha}$ error terms from $R(x)$ as we now verify.

The $\Delta^{n+2+\alpha}$ terms came from E_0 and from the portion

$$\gamma_i[f] = \Delta^{n+3} W_n |s'(\xi_i) f[y_0, ..., y_n, \xi_i]|, \qquad x_i \leq \xi_i \leq x_{i+1},$$

of E_i for $1 \leq i \leq N-1$. When $R(x)$ is substituted for $f(x)$ in E_0 and $\gamma_i[f]$, we get

$$|E_0[R]| \leq \int_0^\Delta |s(x) R[y_0, ..., y_n, x] w_n(x)| \, dx$$

$$\leq \Delta^{n+1} \int_0^\Delta |s(x) R^{(n+1)}(\xi(x))| \, dx/(n+1)!, \qquad 0 \leq \xi(x) \leq \Delta$$

and

$$\gamma_i[R] = \Delta^{n+3} W_n |s'(\xi_i) R^{(n+1)}(\bar{\xi}_i(\xi_i))|/(n+1)!,$$
$$x_i \leq \bar{\xi}_i(\xi_i) \leq x_{i+1}, \qquad 1 \leq i \leq N-1.$$

Now $f^{(n+1)}(x) = f^{(n+1)}(0) + R^{(n+1)}(x)$ and also, $f^{(n+1)}(x) = f^{(n+1)}(0) + x f^{(n+2)}(\xi)$, $0 \leq \xi \leq x$, so that $|R^{(n+1)}(x)| \leq x M_{n+2}$. Then

$$|E_0[R]| \leq \Delta^{n+3+\alpha} M_{n+2} (1+\alpha)^{-1}/(n+1)!,$$

and

$$|\gamma_i[R]| \leq \Delta^{n+3} W_n M_{n+2} |s'(\xi_i) \bar{\xi}_i(\xi_i)|/(n+1)!$$
$$\leq \Delta^{n+3} W_n M_{n+2} |2\alpha s(\xi_i)|/(n+1)!, \qquad 1 \leq i \leq N-1.$$

Both these estimates lead to $\Delta^{n+3+\alpha}$ terms in the bound on the error in the $(n+1)$-point rule for $\int_0^1 s(x) R(x) \, dx$, but not to $\Delta^{n+2+\alpha}$ terms.

III. Examples of Singular Quadrature Rules

Here, we list the explicit formulas for the more useful lower order rules. We also draw the connection to Davis's rule. We revert to the more general form

$$I = \int_a^b s(x) f(x) \, dx. \tag{3.1}$$

The singularity of $s(x)$ is at an arbitrary point x_s. The interval $[a, b]$ is divided into N subintervals $[x_i, x_{i+1}]$ of width $\Delta = N^{-1}(b-a)$; and $x_i = a + i\Delta$, $0 \leqq i \leqq N$. Then

$$I = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} s(x) f(x)\, dx = \sum_{i=0}^{N-1} I_i. \tag{3.2}$$

To obtain an $(n+1)$th-order modified Newton–Cotes approximation $I_i^{(0)}$ to I_i, the general plan is this:

In interval $[x_i, x_{i+1}]$, we have available the Newton–Cotes nodes y_k, $0 \leqq k \leqq n$, and the associated functional values $f_k = f(y_k)$. Let $m_i = \frac{1}{2}(x_i + x_{i+1})$ denote the mid-point of the interval. The interpolating polynomial $P_n(x)$ for this interval, defined by Eq. (2.4) is first reduced to

$$P_n(x) = c_0 + c_1(x - m_i) + c_2(x - m_i)^2 + \cdots + c_n(x - m_i)^n. \tag{3.3}$$

This, in turn, is reexpressed as

$$P_n(x) = C_0 + C_1(x - x_s) + C_2(x - x_s)^2 + \cdots + C_n(x - x_s)^n. \tag{3.4}$$

By setting $x - m_i = z$ and $x - x_s = z + (m_i - x_s)$ and comparing powers of z, we get the C's expressed recursively in terms of the c's. The C's depend linearly on the functional values f_k in the interval and also depend on powers of $(m_i - x_s)$. Then the quadrature rule for I_i takes the form

$$I_i^{(0)} = \int_{x_i}^{x_{i+1}} P_n(x)\, s(x)\, dx = \sum_{k=0}^{n} C_k \int_{x_i}^{x_{i+1}} (x - x_s)^k\, s(x)\, dx. \tag{3.5}$$

To apply the $(n+1)$th-order rule, the indefinite integrals of $(x - x_s)^k\, s(x)$ must be available, preferably in analytic form, and $f(x)$ should be of class $C^{n+2}[a, b]$ for even n and of class $C^{n+1}[a, b]$ for odd n.

A. *Enumeration of Rules*

(1) Modified midpoint rule (open 1-point rule, $n = 0$, $y_0 = m_i$),

$$I_i^{(0)} = f(m_i) \int_{x_i}^{x_{i+1}} s(x)\, dx.$$

(2) Modified trapezoidal rule (closed 2-point rule, $n = 1$, $y_0 = x_i$, $y_1 = x_{i+1}$). Apply (3.5) with

$$C_1 = \Delta^{-1}(f_1 - f_0)$$

$$C_0 = \tfrac{1}{2}(f_1 + f_0) - C_1(m_i - x_s).$$

(3) Modified Simpson's rule (closed 3-point rule, $n=2$, $y_0=x_i$, $y_1=m_i$, $y_2=x_{i+1}$). Apply (3.5) with

$$C_2=\Delta^{-2}(2f_2-4f_1+2f_0)$$
$$C_1=\Delta^{-1}(f_2-f_0)-2(m_i-x_s)\,C_2$$
$$C_0=f_1-(m_i-x_s)^2\,C_2-(m_i-x_s)\,C_1.$$

(4) Modified 4-point rule (closed 4-point rule, $n=3$, $y_k=x_i+k\Delta/3$, $0\leqq k\leqq 3$). Apply (3.5) with

$$C_3=(9/2)\,\Delta^{-3}\,(f_3-3f_2+3f_1-f_0),$$
$$C_2=(9/4)\,\Delta^{-2}(f_3-f_2-f_1+f_0)-3(m_i-x_s)\,C_3,$$
$$C_1=(1/8)\,\Delta^{-1}\,(-f_3+27f_2-27f_1+f_0)-3(m_i-x_s)^2\,C_3-2(m_i-x_s)\,C_2,$$
$$C_0=(1/16)(-f_3+9f_2+9f_1-f_0)-(m_i-x_s)^3\,C_3-(m_i-x_s)^2\,C_2-(m_i-x_s)\,C_1.$$

B. *Relation of Davis's Rule to the Modified Midpoint Rule*

Davis's rule applies to integrals of the type

$$I(a,b)=\int_a^b \prod_{k=1}^{K}(x-d_k)^{\alpha_k}\,dx. \tag{3.6}$$

The integral is approximated as a sum of integrals over subintervals of common length:

$$I(a,b)=\sum_i I(x_i,x_{i+1}),\qquad x_{i+1}-x_i=\Delta, \tag{3.7a}$$

and on each subinterval,

$$I(x_{i+1},x_i)\approx\Delta\prod_{k=1}^{K}\left[\Delta^{-1}\int_{x_i}^{x_{i+1}}(x-d_k)^{\alpha_k}\,dx\right]. \tag{3.7b}$$

Now the average of any function $f(x)$ of class C^2 on (x_i,x_{i+1}) is approximated by its midpoint value $f(m_i)$ to relative order Δ^2. More precisely,

$$\Delta^{-1}\int_{x_i}^{x_{i+1}}f(x)\,dx=f(m_i)+(\Delta^2/24)\,f''(\xi_i),\qquad x_i<\xi_i<x_{i+1}. \tag{3.8}$$

It follows that on any interval (a,b) on which $s(x)$ is singular and $f_k(x)$, $k=1,2,\ldots$, are of class $C^2[a,b]$, the approximation

$$\int_a^b s(x)\prod_k f_k(x)\,dx=\sum_i\left[\int_{x_i}^{x_{i+1}}s(x)\,dx\prod_k\Delta^{-1}\int_{x_i}^{x_{i+1}}f_k(x)\,dx\right] \tag{3.9}$$

differs from the modified midpoint rule only by error terms of order Δ^2, and so has the same order of error from the exact integral as the midpoint rule. The approximation (3.7) to (3.6) is a special case of this. The interval may be divided into K segments, with each segment containing one singularity. The end points of these segments may be chosen, for example, midway between the singularities. On each segment, all but one of the $(x-d_k)^{\alpha_k}$ is of class C^2 and the error terms identified in Section II above, are relevant.

The Davis rule has the advantage, with respect to computer programming, that a single general form represents the approximate integral over a subinterval, regardless of the subinterval's location relative to singularities. If one of the other rules is used, higher accuracy for a given subinterval size is gained, but the convenience of a single general form for the approximating function is lost.

IV. Numerical Examples

A. *A Straightforward Integral*

We check the error estimates of Section II by evaluating numerically the integral

$$I=\int_0^1 x^\alpha e^{-x}\,dx \tag{4.1}$$

in the range $-1<\alpha\leqq 1$. The value of this integral to machine accuracy (e.g., 14 figures) might be found, for example, by integrating by parts five times and applying the standard Simpson's rule with 2000 integration steps. Each of the modified rules of Section III.A leads to an approximate value $I^{(0)}$ and an absolute error $E=|I-I^{(0)}|$.

Results for the modified midpoint rule are shown in Fig. 1. We note that when $s(x)$ remains finite in $[0, 1]$, the modified rule retains the Newton–Cotes rate of convergence ($\alpha=0.5$, $E/I\sim\Delta^{2.0}$). Presence of a stronger singularity degrades the rate of convergence to $E/I\sim\Delta^{2+\alpha}$, as predicted in Section II, and increases the absolute value of the error.

Results for different modified rules for the case of $\alpha=-0.9$ are displayed in Fig. 2. The predicted rate of convergence $\Delta^{n+2+\alpha}$ for n even (midpoint and Simpson's) is clearly reproduced. The predicted rate of convergence for n odd depends on whether $\Delta>\Delta_c$ or $\Delta<\Delta_c$. Since $\Delta_c=4.5\times10^{-5}$, the expected rate of convergence for the values of Δ shown in Fig. 2 is $\Delta^{n+1}\log(\Delta^{-1})$. This slight deterioration from the Newton–Cotes rate convergence of Δ^{n+1} can be qualitatively seen in the case of the modified trapezoidal rule (Fig. 2). However, it is barely seen in the case of the modified four-point rule due to its rapid convergence.

We note, as a general conclusion, the fact that modified rules of odd order have a convergence rate very close to the Newton–Cotes rules, while modified rules of even

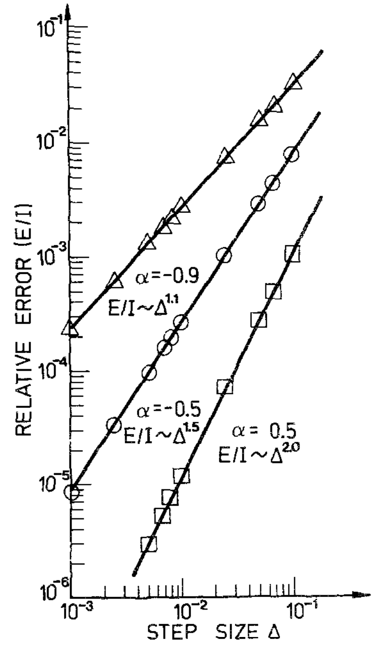

FIG. 1. Relative error of the modified midpoint rule for singularity $s(x) \sim x^{\alpha}$, as a function of singularity strength and integration step. See Section IV.A.

order may lose up to one order in the rate of convergence as compared to the Newton–Cotes rules, depending on the strength of singularity.

B. *A More Difficult Example*

Consider the following integral of Schwarz–Christoffel type:

$$I = \int_0^1 (x + 0.001)^{-0.9} x^{-0.9} (1.01 - x)^{-0.9}\, dx. \tag{4.2}$$

This integral presents a greater challenge to approximation methods because several strong, closely spaced singularities are present. We first suggest that the integration interval be decomposed into subintervals such that (a) no subinterval contains more than one singularity and (b) the minimum distance from a subinterval to the nearest singularity external to it is not less than one-fifth to one-tenth the subinterval width. In each subinterval, $s(x)$ will represent the interior singularity, if there is one, and the nearest external singularity otherwise. This guideline, based on our numerical experimentation in a variety of cases, may not be optimal, but is certainly quite serviceable.

Following this plan, we divide $(0, 1)$ into four subintervals: $(0, 0.005)$,

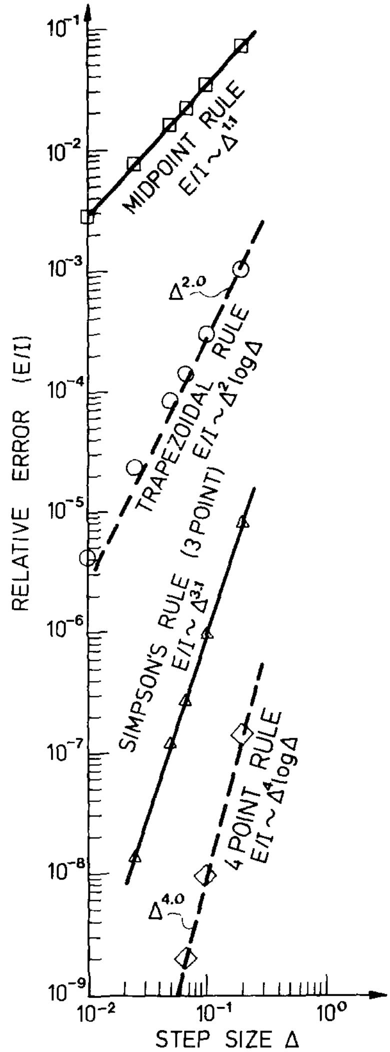

FIG. 2. Relative error of various modified Newton–Cotes singular quadrature rules for singularity $s(x) \sim x^{-0.9}$. See Section IV.A.

(0.005, 0.05), (0.05, 0.9), and (0.9, 1). The integral over each subinterval was then calculated by the composite Davis rule, the composite 4-point rule, and the Gauss–Jacobi rule, and the results totaled to get Davis, 4-point, and Gauss–Jacobi estimates of I. "Composite" means that each subinterval was itself subdivided into N parts, and the relevant rule applied to that part. For Gauss–Jacobi, an Nth order rule was applied separately to each of the four subintervals.

Table I shows error data on the 3 rules for values of N varying by powers of 2 up

TABLE I

Relative Effectiveness of Various Quadrature Rules for a Difficult Singular Integral of the Schwarz–Christoffel Type (see Section IV.B)

	Davis rule			4-point rule			Gauss–Jacobi		
N	Nodes	Error	t	Nodes	Error	t	Nodes	Error	t
1				13	0.016	0.001	4	0.18	0.004
2				25	0.0043	0.001	8	0.030	0.004
4				49	8.3×10^{-4}	0.002	16	0.0018	0.007
8	32	0.15	0.001	97	1.1×10^{-4}	0.003	32	2.8×10^{-5}	0.020
16	64	0.083	0.002	193	1.1×10^{-5}	0.005	64	1.7×10^{-8}	0.062
32	128	0.042	0.004	385	8.8×10^{-7}	0.011	128	2.5×10^{-13}	0.204
64	256	0.021	0.008	769	6.3×10^{-8}	0.021			
128	512	0.0099	0.015	1537	4.2×10^{-9}	0.041			
256	1024	0.0047	0.030	3073	2.8×10^{-10}	0.082			
1024	4096	0.0010	0.118						

to 1024. For each rule and various N, Table I shows the total number of nodes at which evaluations of $f(x)$ are made, the relative error, and the computing time in seconds (for a Cray 1).

The Davis rule is the simplest to program, but is significantly less effective than the other two. It would have looked relatively better if positive values, rather than -0.9 had been chosen for the singularity exponents.

The Gauss–Jacobi quadrature is more effective than the 4-point rule in terms of the number of functional evaluations needed for a given accuracy level, by a factor of the order of 6 to 12, but less effective in terms of computer time required for a given accuracy level by a factor of the order of 3 or 4 for a range of cases. But note that the quoted Gauss–Jacobi computer time includes the cost of computing the nodes and weights; in an iterative calculation with many integrations, but few recalculations of nodes and weights, the comparative Gauss–Jacobi times could be significantly improved. Then again, the modified 4-point rule, and the other listed modified Newton–Cotes rules, are almost as routine to program as the Davis rule.

We do not conclude that any one of the rules examined is always the best; each has its advantages depending on the specific problem.

We do expect that the rules developed in this paper can find wide application as efficient, easily programmed, singular quadrature rules for a variety of problems.

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