MATHEMATICS OF COMPUTATION
VOLUME 56, NUMBER 194
APRIL 1991, PAGES 741-754

AN AUTOMATIC QUADRATURE FOR CAUCHY PRINCIPAL VALUE INTEGRALS

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ABSTRACT. An automatic quadrature is presented for computing Cauchy principal value integrals $Q(f; c) = ⨍_a^b f(t)/(t-c)\,dt$, $a < c < b$, for smooth functions $f(t)$. After subtracting out the singularity, we approximate the function $f(t)$ by a sum of Chebyshev polynomials whose coefficients are computed using the FFT. The evaluations of $Q(f; c)$ for a set of values of c in (a, b) are efficiently accomplished with the same number of function evaluations. Numerical examples are also given.

1. INTRODUCTION

We present an automatic quadrature scheme for approximating principal value integrals

$$(1.1)\qquad Q(f; c) = ⨍_{-1}^{1} \frac{f(t)}{t-c}\,dt, \qquad -1 < c < 1,$$

where $f(t)$ are assumed to be smooth functions. Piessens et al. [17] give an automatic quadrature program for evaluating $Q(f; c)$ in (1.1) for a single value of c.

In this paper, for a set of values of c in $(-1, 1)$ we efficiently compute a set of approximations $\{Q_N(f; c)\}$ to the integrals (1.1) satisfying the prescribed tolerance ε_a. To this end, it is required to construct quadrature rules which have error estimates independent of the values of c for smooth functions $f(t)$.

Our method is an extension of the Clenshaw-Curtis method [4] (henceforth abbreviated to CC method) for the integral $\int_{-1}^{1} f(t)\,dt$ to the problem (1.1) [1], [2], [3], [14]. In the CC method, the function $f(t)$ is approximated by a sum of Chebyshev polynomials $T_k(t)$,

$$(1.2)\qquad p_N(t) = \sum_{k=0}^{N}{}'' a_k^N\, T_k(t), \qquad -1 \le t \le 1,$$

Received October 30, 1989.
1980 *Mathematics Subject Classification* (1985 *Revision*). Primary 65D30, 65D32; Secondary 41A55.
Key words and phrases. Cauchy principal value integral, automatic integration, Chebyshev interpolation.

interpolating $f(t)$ at the abscissae $t_j^N = \cos(\pi j/N)$ $(0 \le j \le N)$, which are the zeros of the polynomial $\omega_{N+1}(t)$ defined by

$$(1.3) \qquad \omega_{N+1}(t) = T_{N+1}(t) - T_{N-1}(t) = 2\,(t^2 - 1)\,U_{N-1}(t), \qquad N \ge 1,$$

where $U_k(t)$ is the Chebyshev polynomial of the second kind defined by $U_k(t) = \sin(k+1)\theta/\sin\theta$ $(t = \cos\theta)$. In (1.2), the double prime denotes the summation where the first and last terms are halved. The truncated Chebyshev series (1.2) converges rapidly as N increases if $f(t)$ is a smooth function.

Chawla and Kumar [3] substituted $p_N(t)$ (1.2) for $f(t)$ in (1.1) to obtain an approximation $Q_N^{CK}(f; c)$ to $Q(f; c)$ as follows:

$$(1.4) \qquad Q_N^{CK}(f; c) = \sum_{k=0}^{N}{}'' a_k^N Q(T_k; c),$$

where the modified moment $Q(T_k; c) = ⨍_{-1}^{1} T_k(t)/(t - c)\,dt$ can be computed by means of a three-term recurrence relation [1]. However, this method is not suitable for our purpose because the error $Q(f; c) - Q_N^{CK}(f; c)$ cannot be bounded independently of the value of c [3].

On the other hand, subtracting out the singularity [5, p.184], [7, p.104], [18], [19], one can write $Q(f; c)$ (1.1) in the form

$$(1.5) \qquad Q(f; c) = \int_{-1}^{1} g_c(t)\,dt + f(c)\,\log\left(\frac{1-c}{1+c}\right),$$

where $g_c(t)$ is defined by

$$(1.6) \qquad g_c(t) = \{f(t) - f(c)\}/(t - c).$$

Chawla and Jayarajan [2], and subsequently Kumar [14], made use of the approximate polynomial $p_N(t)$ (1.2) to interpolate $g_c(t)$ instead of $f(t)$ at t_j^N and obtained the quadrature formulae

$$(1.7) \qquad Q_N^{CJ}(f; c) = \sum_{j=0}^{N}{}'' A_j^N g_c(t_j^N) + f(c)\,\log\left(\frac{1-c}{1+c}\right),$$

when $t_j^N \ne c$ for all j. In the above, A_j^N are given by

$$A_j^N = \frac{4}{N}\sum_{k=0}^{N/2}{}'' T_{2k}(t_j^N)/(1 - 4k^2), \qquad 0 \le j \le N,$$

where here and henceforth we conveniently assume that N is even.

It is known [14] that the quadrature formulae (1.7) can yield, in general, better approximate values for (1.1) than the formulae (1.4), but in the computation of $g_c(t_j^N)$, we have severe numerical cancellation if a node t_j^N happens to be very close to c [9], [15]. This instability requires special care in programming the function g_c.

We now show that we can avoid this instability by approximating $f(t)$ and $f(c)$ in (1.6) by $p_N(t)$ and $p_N(c)$ (1.2), respectively; the approximation $Q_N(f;c)$ to the integral $Q(f;c)$ then becomes

$$Q_N(f;c) = \int_{-1}^{1} \frac{p_N(t)-p_N(c)}{t-c}\,dt + f(c)\log\left(\frac{1-c}{1+c}\right). \tag{1.8}$$

Expanding the integrand in (1.8) in Chebyshev polynomials,

$$\frac{p_N(t)-p_N(c)}{t-c} = {\sum_{k=0}^{N-1}}' d_k\, T_k(t), \tag{1.9}$$

and integrating term by term, yields a new integration formula

$$Q_N(f;c) = 2 {\sum_{k=0}^{N/2-1}}' d_{2k}/(1-4k^2) + f(c)\log\left(\frac{1-c}{1+c}\right), \tag{1.10}$$

where the prime denotes the summation whose first term is halved. The coefficients d_k in (1.9) can be stably computed by using the recurrence relation

$$d_{k+1} - 2c\,d_k + d_{k-1} = 2a_k^N, \qquad k = N, N-1, \dots, 1, \tag{1.11}$$

in the backward direction with the starting values $d_N = d_{N+1} = 0$, where we take $a_N^N/2$ instead of a_N^N. We have omitted the dependence of d_k on N and c.

It is well known that the Fast Fourier Transform (FFT) is useful for efficiently computing the coefficients $\{a_k^N\}$ in (1.2); see also (2.1) below, [1] and [10], where by doubling N the computation can be repeated, reusing the previous values until an error criterion is satisfied. It is advantageous to have more chances of checking the stopping criterion than by doubling N, in order to enhance the efficiency of automatic quadrature. In [12], we allowed N to take the forms 3×2^n and 5×2^n as well as 2^n, that is,

$$N = 3, 4, 5, \dots, 3\times 2^n, 4\times 2^n, 5\times 2^n, \dots \; (n = 1, 2, \dots). \tag{1.12}$$

In §2 we briefly review how to generate recursively the sequence of the interpolating polynomials $\{p_N(t)\}$ by increasing N as in (1.12) and by using the FFT. The set of the $N+1$ nodes u_j^N ($0 \le j \le N$) for $p_N(t)$ is chosen to be a subset of $\{\cos \pi j/2^m\}$ ($0 \le j \le 2^m$) used in the CC method, where m is the smallest integer such that $N \le 2^m$.

We remark that the present quadrature rule $Q_N(f;c)$ (1.8) or (1.10) is not of interpolatory type because the degree of exactness in the present rule, using $N+2$ abscissae, u_j^N $(0 \le j \le N)$ and c, is N, not $N+1$. As will be shown in §3, however, since the function value $f(c)$ is used in the quadrature rule $Q_N(f;c)$ (1.8), but not in interpolating $f(t)$, the error of $Q_N(f;c)$ can be bounded independently of the value of c for smooth functions $f(t)$. See (3.8), (3.10), and (3.11) below. This fact enables us to use the polynomial $p_N(t)$ common to the set of the approximations $\{Q_N(f;c)\}$ for a set of c-values in $(-1, 1)$. In §4 numerical comparisons with other automatic quadrature methods are shown.

2. Computation of the Chebyshev coefficients

We will outline the iterative procedure for computing the sequence $\{p_N(t)\}$ (1.2) of the truncated Chebyshev series by increasing N as in (1.12). For details, see [12].

We begin with the sample points for $p_N(t)$ to interpolate $f(t)$. If the sample points are carefully chosen, the interpolating polynomial converges [13, p. 254]. We gave in [11] and [12] a sequence $\{\beta_j\}$ which is a modification of the van der Corput sequence and satisfies the recurrence relation:

$$\beta_{2j} = \beta_j/2, \qquad \beta_{2j+1} = \beta_{2j} + 1/2, \qquad j = 1, 2, \dots,$$

with the starting value $\beta_1 = 3/4$. The set of the sample points $\{\cos 2\pi\beta_j\}$ ($j = -1, 0, 1, \dots$), where we put $\beta_{-1} = 0$ and $\beta_0 = 1/2$, is a sequence of Chebyshev points [13, p. 254], which makes the sequence of interpolating polynomials converge uniformly on $[-1, 1]$ for functions analytic on $[-1, 1]$. The polynomial $p_N(t)$ is determined so as to interpolate $f(t)$ at the first $N+1$ points of the sequence $\{\cos 2\pi\beta_j\}$ ($j = -1, 0, 1, \dots$).

Let $N = 2^n$ ($n = 2, 3, \dots$); then the set of the $N+1$ abscissae $\{\cos 2\pi\beta_j\}$ ($-1 \le j < N$) coincides with the zeros of $\omega_{N+1}(t)$ (1.3), that is, $\{\cos \pi j/N\}$ ($0 \le j \le N$) used in the CC method. Therefore, the interpolation condition

$$p_N(\cos \pi j/N) = f(\cos \pi j/N), \qquad 0 \le j \le N,$$

determines the coefficients a_k^N for $p_N(t)$ (1.2) as follows:

$$a_k^N = \frac{2}{N} \sum_{j=0}^{N}{}'' f(\cos \pi j/N) \cos(\pi k j/N), \quad 0 \le k \le N. \tag{2.1}$$

It is known that the right-hand side of (2.1) can be efficiently computed by means of the FFT for real data [10].

We represent the polynomials $p_{5N/4}(t)$ and $p_{3N/2}(t)$ interpolating $f(t)$ at the nodes $\{\cos 2\pi\beta_j\}$, where $-1 \le j < N + N/4$ for $p_{5N/4}(t)$ and $-1 \le j < N + N/2$ for $p_{3N/2}(t)$, respectively, in the form

$$\begin{aligned} p_{5N/4}(t) - p_N(t) &= -\omega_{N+1}(t) \sum_{k=1}^{N/4} b_k^N U_{k-1}(t) \\ &= \sum_{k=1}^{N/4} b_k^N \{T_{N-k}(t) - T_{N+k}(t)\}, \end{aligned} \tag{2.2}$$

$$
\begin{aligned}
p_{3N/2}(t) - p_N(t) &= -\omega_{N+1}(t) \sum_{k=1}^{N/2} B_k^N U_{k-1}(t) \\
&= \sum_{k=1}^{N/2} B_k^N \{T_{N-k}(t) - T_{N+k}(t)\}.
\end{aligned} \tag{2.3}
$$

Then, the coefficients $\{b_k^N\}$ and $\{B_k^N\}$ are determined to satisfy the conditions

$$
\begin{aligned}
p_{5N/4}(v_j^N) &= f(v_j^N), \qquad 0 \le j < N/4, \\
p_{3N/2}(w_j^N) &= f(w_j^N), \qquad 0 \le j < N/2,
\end{aligned}
$$

where the sample points v_j^N and w_j^N are defined by

$$
v_j^N = \cos 8\pi(j + \beta_4)/N \quad \text{or} \quad T_{N/4}(v_j^N) - \cos 2\pi\beta_4 = 0, \tag{2.4}
$$

$$
w_j^N = \cos 4\pi(j + \beta_2)/N \quad \text{or} \quad T_{N/2}(w_j^N) - \cos 2\pi\beta_2 = 0, \tag{2.5}
$$

respectively. This is because the set of the additional $N/4$ ($N/2$) abscissae $\{\cos 2\pi\beta_j\}$, $N \le j < N/4$ ($N \le j < N/2$) for $p_{5N/4}(t)$ ($p_{3N/2}(t)$) coincides with $\{v_j^N\}$, $0 \le j < N/4$ ($\{w_j^N\}$, $0 \le j < N/2$) [12]. If the set of $N/2$ sample points $\{\cos 4\pi(j+\beta_3)/N\}$ ($0 \le j < N/2$), which agrees with $\{\cos 2\pi\beta_j\}$ ($3N/2 \le j < 2N$), is added to the set of abscissae for $p_{3N/2}(t)$, we have $2N+1$ abscissae $\{\cos \pi j/(2N)\}$ ($0 \le j \le 2N$) for $p_{2N}(t)$. Thus the sequence of the interpolating polynomials $\{p_{3m}(t), p_{4m}(t), p_{5m}(t), \dots\}$ ($m = 2^n$, $n = 1, 2, \dots$) is recursively generated. The FFT [12] is used to efficiently compute the coefficients $\{b_k^N\}$ and $\{B_k^N\}$.

3. Error estimates

Assume that $N = 2^n$ ($n = 2, 3, \dots$) and define A_k^N by

$$
A_k^N = \begin{cases} a_k^N, & 0 \le k < N - N/4, \\ a_k^N + b_{N-k}^N, & N - N/4 \le k < N, \\ a_N^N/2, & k = N, \\ -b_{k-N}^N, & N < k \le N + N/4. \end{cases} \tag{3.1}
$$

Then, the approximate quadrature $Q_{5N/4}(f; c)$ depending on the polynomial $p_{5N/4}(t)$ (2.2) is given by the right-hand side of (1.10), where the sum ranges from 0 to $N/2 + N/8 - 1$, and by (1.11) with a_k^N replaced by A_k^N (3.1). Similarly, one can obtain the approximation $Q_{3N/2}(f; c)$ depending on the polynomial $p_{3N/2}(t)$ (2.3).

Now, we will give error estimates for the approximations $Q_N(f; c)$, $Q_{5N/4}(f; c)$, and $Q_{3N/2}(f; c)$, especially for analytic functions f. Let

ε_ρ denote the ellipse in the complex plane $z = x + iy$ with foci $(x, y) = (-1, 0), (1, 0)$ and semimajor axis $a = (\rho + \rho^{-1})/2$ and semiminor axis $b = (\rho - \rho^{-1})/2$ for a constant $\rho > 1$.

Assume that $f(z)$ is single-valued and analytic inside and on ε_ρ. Then, the error of the interpolating polynomial $p_N(t)$ can be expressed in terms of a contour integral [6], [7, p. 105], [8], which is also expanded in a Chebyshev series [11]:

$$(3.2)\qquad f(t) - p_N(t) = \frac{1}{2\pi i}\oint_{\varepsilon_\rho} \frac{\omega_{N+1}(t)\, f(z)\, dz}{(z-t)\,\omega_{N+1}(z)} = \omega_{N+1}(t) \sideset{}{'}\sum_{k=0}^{\infty} V_k^N(f)\, T_k(t),$$

where the coefficients $V_k^N(f)$ are given by

$$(3.3)\qquad V_k^N(f) = \frac{1}{\pi^2 i}\oint_{\varepsilon_\rho} \frac{\widetilde{U}_k(z) f(z)\, dz}{\omega_{N+1}(z)}, \qquad k \geq 0.$$

The Chebyshev function of the second kind, $\widetilde{U}_k(z)$, is defined by

$$(3.4)\qquad \widetilde{U}_k(z) = \int_{-1}^{1} \frac{T_k(t)\, dt}{(z-t)\sqrt{1-t^2}} = \frac{\pi}{\sqrt{z^2-1}\, w^k} = \frac{2\pi}{(w - w^{-1})\, w^k},$$

where $w = z + \sqrt{z^2 - 1}$ and $|w| > 1$ for $z \notin [-1, 1]$ [8], [11].

Using (3.2) in (1.5), (1.6) and (1.8) yields the error for the approximate integral $Q_N(f; c)$:

$$(3.5)\qquad Q(f; c) - Q_N(f; c) = \sideset{}{'}\sum_{k=0}^{\infty} \Omega_k^N(c)\, V_k^N(f),$$

where $\Omega_k^N(c)$ is given by

$$(3.6)\qquad \Omega_k^N(c) = \int_{-1}^{1} \frac{\omega_{N+1}(t)\, T_k(t) - \omega_{N+1}(c)\, T_k(c)}{t - c}\, dt, \qquad k \geq 0.$$

In Appendix A we prove the following lemma.

Lemma 3.1. *Let $N = 2^n$, $n = 2, 3, \ldots$, and $\Omega_k^N(c)$ be defined by (3.6). Then, $\Omega_k^N(c)$ is bounded independently of the value of c as well as N and k; indeed,*

$$(3.7)\qquad |\Omega_k^N(c)| \leq 8.$$

From (3.5) and (3.7) we have the following theorem.

Theorem 3.2. *Let $N = 2^n$, $n = 2, 3, \ldots$, and assume that $f(z)$ is single-valued and analytic inside and on ε_ρ. Then, the error of the approximate integral $Q_N(f; c)$ given by (1.10) is bounded independently of c by*

$$(3.8)\qquad |Q(f; c) - Q_N(f; c)| \leq 8 \sideset{}{'}\sum_{k=0}^{\infty} |V_k^N(f)|,$$

where $V_k^N(f)$ is given by (3.3).

Similarly, the errors of the approximate integrals $Q_{5N/4}(f;c)$ and $Q_{3N/2}(f;c)$ are bounded as follows:

Theorem 3.3. *Let* $N = 2^n$ $(n = 2, 3, \ldots)$ *and assume that* $f(z)$ *is single-valued and analytic inside and on* ε_ρ. *Further, let* $V_k^{N+N/\sigma}(f)$ $(\sigma = 2, 4)$ *be defined by*

$$V_k^{N+N/\sigma}(f) = \frac{1}{\pi^2 i} \oint_{\varepsilon_\rho} \frac{\widetilde{U}_k(z) f(z)\, dz}{\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}}, \quad k \geq 0, \quad \sigma = 2, 4. \tag{3.9}$$

Then, we have

$$\begin{aligned} |Q(f;c) - Q_{5N/4}(f;c)| &\leq 8\,(1 + |\cos 2\pi\beta_4|) \sideset{}{'}\sum_{k=0}^{\infty} |V_k^{N+N/4}(f)| \\ &\sim 11.1 \sideset{}{'}\sum_{k=0}^{\infty} |V_k^{N+N/4}(f)|, \end{aligned} \tag{3.10}$$

$$\begin{aligned} |Q(f;c) - Q_{3N/2}(f;c)| &\leq 8\,(1 + |\cos 2\pi\beta_2|) \sideset{}{'}\sum_{k=0}^{\infty} |V_k^{N+N/2}(f)| \\ &\sim 13.7 \sideset{}{'}\sum_{k=0}^{\infty} |V_k^{N+N/2}(f)|, \end{aligned} \tag{3.11}$$

where $\beta_4 = 3/16$ *and* $\beta_2 = 3/8$.

Proof. The error of the interpolating polynomial $p_{N+N/\sigma}(t)$ $(\sigma = 2, 4)$ has an expression similar to (3.2):

$$\begin{aligned} f(t) - p_{N+N/\sigma}(t) &= \frac{1}{2\pi i} \oint_{\varepsilon_\rho} \frac{\omega_{N+1}(t)\{T_{N/\sigma}(t) - \cos 2\pi\beta_\sigma\} f(z)\, dz}{(z-t)\,\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}} \\ &= \omega_{N+1}(t)\{T_{N/\sigma}(t) - \cos 2\pi\beta_\sigma\} \\ &\quad \times \sideset{}{'}\sum_{k=0}^{\infty} V_k^{N+N/\sigma}(f)\, T_k(t), \qquad \sigma = 2, 4, \end{aligned} \tag{3.12}$$

where $V_k^{N+N/\sigma}(f)$ is given by (3.9). If we note in (3.12) that

$$\begin{aligned} &2\,\omega_{N+1}(t)\{T_{N/\sigma}(t) - \cos 2\pi\beta_\sigma\} \\ &\quad = \omega_{N+N/\sigma+1}(t) + \omega_{N-N/\sigma+1}(t) - 2\cos 2\pi\beta_\sigma\, \omega_{N+1}(t), \end{aligned} \tag{3.13}$$

then the proof of (3.10) and (3.11) is established in a way similar to that for (3.8). □

Suppose that $f(z)$ is a meromorphic function which has M simple poles at the points z_m $(m = 1, 2, \ldots, M)$ outside of ε_ρ with residues $\operatorname{Res} f(z_m)$.

Then, performing the contour integral of (3.3) gives

$$V_k^N(f) = -\frac{2}{\pi}\sum_{m=1}^{M} \operatorname{Res} f(z_m)\,\widetilde{U}_k(z_m)/\omega_{N+1}(z_m), \qquad k \geq 0. \tag{3.14}$$

Put $z = (w + w^{-1})/2$; then the Chebyshev polynomial can be expressed as

$$T_n(z) = (w^n + w^{-n})/2, \quad w = z + \sqrt{z^2 - 1}, \qquad |w| > 1 \text{ for } z \notin [-1, 1]. \tag{3.15}$$

From (1.3), (3.4), (3.14) and (3.15) it is seen that $|V_k^N(f)| = O(r^{-k-N})$, where $r = \min_{1\leq m\leq M} |z_m + \sqrt{z_m^2 - 1}| > 1$. Thus, from (3.8) we may estimate the error for $Q_N(f; c)$ as follows:

$$|Q(f; c) - Q_N(f; c)| \lesssim 4\,|V_0^N(f)|(r+1)/(r-1). \tag{3.16}$$

Now, we wish to estimate $|V_0^N(f)|$ in terms of the available coefficients a_k^N of the truncated Chebyshev series $p_N(t)$ (1.2). Elliott [6] gives the expression

$$a_k^N = \frac{2}{\pi i}\oint_{\varepsilon_\rho} \frac{T_{N-k}(z)\,f(z)}{\omega_{N+1}(z)}\,dz, \qquad 0 \leq k \leq N. \tag{3.17}$$

Performing the contour integral in (3.17) and comparing with (3.14) gives the estimates

$$|V_0^N| \sim |a_N^N|\,r/(r^2 - 1) \tag{3.18}$$

and $|a_k^N| \sim r\,|a_{k+1}^N|$, unless the poles z_m of $f(z)$ are close to the segment $[-1, 1]$ on the real axis. Finally, from (3.16) and (3.18) we could obtain an estimate of the truncation error $E_N(f; c)$ for $Q_N(f; c)$ as follows:

$$E_N(f; c) = 8\,(|a_N^N|/2)\,r/(r-1)^2, \tag{3.19}$$

where we note that $a_N^N/2$ is the coefficient of the last term in the truncated Chebyshev series (1.2). The constant r may be estimated from the asymptotic behavior of $\{a_k^N\}$ in a way similar to that in the stopping criterion described in [12].

If $|a_k^N|$ decreases slowly as k increases, that is, $r \to 1+$, we prefer a rather cautious error estimation similar to that given in the stopping criterion of [12] in place of (3.19). See also [16].

Next, we turn to estimate the error (3.10) of $Q_{5N/4}(f; c)$ in terms of the available coefficients b_k^N of $p_{5N/4}(t)$ (2.2).

Lemma 3.4. *Let $f(z)$ be single-valued and analytic inside and on ε_ρ. Further, define*

$$J_k^N(\sigma) = \frac{-1}{\pi i}\oint_{\varepsilon_\rho} \frac{T_{N/\sigma-k}(z)\,f(z)\,dz}{\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}}, \qquad 1 \leq k \leq N/\sigma,\ \sigma = 2, 4, \tag{3.20}$$

where the right-hand side of (3.20) *is multiplied by* $1/2$ *when* $k = N/\sigma$. *Then, for* b_k^N *in* (2.2) *and* B_k^N *in* (2.3), *we have* $b_k^N = J_k^N(4)$ *and* $B_k^N = J_k^N(2)$, *respectively.*

Proof. From (3.2) and (3.12) we have

$$(3.21)\quad \begin{aligned} p_{N+N/\sigma}(t) - p_N(t) &= \frac{1}{2\pi i}\oint_{\mathcal{E}_\rho} \frac{\omega_{N+1}(t)\{T_{N/\sigma}(z) - T_{N/\sigma}(t)\} f(z)\,dz}{(z-t)\,\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}} \\ &= \frac{1}{\pi i}\sum_{n=0}^{N/\sigma-1}{}' \oint_{\mathcal{E}_\rho} \frac{\omega_{N+1}(t)\,U_{N/\sigma-n-1}(t)\,T_n(z)\,f(z)\,dz}{\omega_{N+1}(z)\{T_{N/\sigma}(z) - \cos 2\pi\beta_\sigma\}}, \\ &\qquad \sigma = 2, 4. \end{aligned}$$

In deriving the second equality above we have used the identity (A.3) in Appendix A, where we take N/σ, a complex z and real t for $k+1$, t, and c, respectively. Comparing (2.2), (2.3) and (3.21) establishes Lemma 3.4. □

Performing the contour integrals in (3.9) and (3.20) and comparing both results yields the estimates

$$(3.22)\qquad |V_0^{N+N/4}| \sim 4\,|b_{N/4}^N|\,r/(r^2 - 1),$$

$|V_k^{N+N/4}(f)| = O(r^{-k-N-N/4})$ and $|b_k^N| \sim r\,|b_{k+1}^N|$. Using these relations in (3.10), one gets an estimate of the truncation error $E_{N+N/4}(f; c)$ for $Q_{5N/4}(f; c)$ as follows:

$$(3.23)\qquad E_{5N/4}(f; c) = 22.2\,|b_{N/4}^N|\,r/(r-1)^2.$$

Similarly, it follows that

$$(3.24)\qquad E_{3N/2}(f; c) = 27.4\,|B_{N/2}^N|\,r/(r-1)^2.$$

If the constant r is found to be close or equal to 1, we resort to a check procedure; see the stopping criterion in [12].

It should be noted that the error estimates (3.19), (3.23) and (3.24) for the quadrature rules $Q_N(f; c)$, $Q_{5N/4}(f; c)$, and $Q_{3N/2}(f; c)$, respectively, are independent of the value of c. This fact enables us to use the approximate polynomial $p_N(t)$, $p_{5N/4}(t)$ or $p_{3N/2}(t)$ common to the set of the integrals $Q(f; c)$ (1.1) for a set of c-values if a stopping criterion is satisfied.

4. Numerical examples

We now show numerical results obtained with the present automatic quadrature scheme for the following test problems:

$$\fint_{-1}^{1} \frac{\exp\{a(t-1)\}}{t-c}\,dt, \qquad a = 4, 8, 16, \tag{4.1}$$

$$\fint_{-1}^{1} \frac{(t^2+a^2)^{-1}}{t-c}\,dt, \qquad a = 1, 1/4, 1/8, \tag{4.2}$$

$$\fint_{0}^{1} \frac{\cos 2\pi a t}{t-c}\,dt, \qquad a = 8, 16, 32, \tag{4.3}$$

$$\fint_{-1}^{1} \frac{1-a^2}{1-2at+a^2}\cdot\frac{1}{t-c}\,dt, \qquad a = 0.8, 0.9, 0.95, \tag{4.4}$$

$$\fint_{0}^{1} \frac{\sqrt{1-t^2}}{t-c}\,dt. \tag{4.5}$$

Table 1

Comparison of the performance of the present method with QAWC in QUADPACK [17] *for* $\fint_{-1}^{1} e^{a(t-1)}/(t-c)\,dt$, $a = 4, 8, 16$. *N denotes the number of abscissae required to satisfy the tolerance* ε_a. *The present method computes all the integrals for a set of the values of c by using* $N-1$ *abscissae once and for all, and by using the number of the corresponding values of c.*

		$\varepsilon_a = 10^{-6}$				$\varepsilon_a = 10^{-10}$			
		present method		QUADPACK		present method		QUADPACK	
a	c	N	error	N	error	N	error	N	error
4	0.2	$\Uparrow^{(+1)}$	1×10^{-10}	25	2×10^{-15}	$\Uparrow^{(+1)}$	9×10^{-15}	105	3×10^{-13}
	0.5	**17+1**	2×10^{-11}	25	4×10^{-15}	**21+1**	1×10^{-16}	105	4×10^{-14}
	0.95	$\Downarrow_{(+1)}$	6×10^{-11}	25	1×10^{-14}	$\Downarrow_{(+1)}$	2×10^{-14}	105	2×10^{-13}
8	0.2	$\Uparrow^{(+1)}$	5×10^{-10}	105	7×10^{-13}	$\Uparrow^{(+1)}$	9×10^{-13}	145	7×10^{-13}
	0.5	**21+1**	3×10^{-10}	105	2×10^{-15}	**25+1**	3×10^{-13}	185	4×10^{-13}
	0.95	$\Downarrow_{(+1)}$	8×10^{-11}	65	4×10^{-15}	$\Downarrow_{(+1)}$	1×10^{-12}	145	2×10^{-13}
16	0.2	$\Uparrow^{(+1)}$	7×10^{-13}	105	7×10^{-13}	$\Uparrow^{(+1)}$	7×10^{-13}	185	7×10^{-13}
	0.5	**33+1**	6×10^{-13}	145	8×10^{-13}	**33+1**	6×10^{-13}	225	8×10^{-13}
	0.95	$\Downarrow_{(+1)}$	2×10^{-14}	105	6×10^{-16}	$\Downarrow_{(+1)}$	2×10^{-14}	185	1×10^{-13}

TABLE 2

Comparison of the performance of the present method with QAWC in QUADPACK [17] *for* $⨍_{-1}^{1} (t^2+a^2)^{-1}/(t-c)\,dt$, $a = 1, 1/4, 1/8$.

		$\varepsilon_a = 10^{-6}$				$\varepsilon_a = 10^{-10}$			
		present method		QUADPACK		present method		QUADPACK	
a	c	N	error	N	error	N	error	N	error
	0.2	$\Uparrow^{(+1)}$	1×10^{-8}	65	4×10^{-13}	$\Uparrow^{(+1)}$	6×10^{-13}	145	4×10^{-13}
1	0.5	**21**+**1**	1×10^{-8}	65	5×10^{-13}	**33**+**1**	5×10^{-13}	145	5×10^{-13}
	0.95	$\Downarrow_{(+1)}$	4×10^{-9}	65	5×10^{-13}	$\Downarrow_{(+1)}$	1×10^{-13}	105	7×10^{-13}
	0.2	$\Uparrow^{(+1)}$	3×10^{-7}	225	2×10^{-11}	$\Uparrow^{(+1)}$	7×10^{-13}	365	3×10^{-12}
1/4	0.5	**81**+**1**	3×10^{-8}	215	9×10^{-12}	**129**+**1**	5×10^{-13}	325	3×10^{-12}
	0.95	$\Downarrow_{(+1)}$	9×10^{-10}	165	1×10^{-11}	$\Downarrow_{(+1)}$	1×10^{-13}	235	2×10^{-12}
	0.2	$\Uparrow^{(+1)}$	4×10^{-7}	335	6×10^{-12}	$\Uparrow^{(+1)}$	1×10^{-12}	505	1×10^{-11}
1/8	0.5	**161**+**1**	3×10^{-7}	225	3×10^{-11}	**257**+**1**	2×10^{-13}	445	1×10^{-12}
	0.95	$\Downarrow_{(+1)}$	1×10^{-7}	255	5×10^{-12}	$\Downarrow_{(+1)}$	5×10^{-13}	325	1×10^{-11}

Tables 1 – 5 compare the results of the present scheme with those of QAWC in the subroutine package QUADPACK [17] for each problem (4.1)–(4.5). We show the number of function evaluations N required to satisfy the requested absolute accuracy ε_a for each integral and the actual errors.

It should be noted that the present scheme can efficiently give all the approximations to the integrals (1.1) for a set of c-values by using the common number of function evaluations once and for all, except for each function value $f(c)$ at c, for smooth functions $f(t)$. Consequently, in each Table 1–5, the present method requires only N + extra 2 ($= N+2$) function evaluations to compute the three integrals for the three values of c. For example, in Table 1, 20 $\{= N+2 = (17+1)+2\}$ function evaluations are sufficient for the three integrals with the parameter $a = 4$ to satisfy the tolerance $\varepsilon_a = 10^{-6}$.

The computation was carried out in double-precision arithmetic (about 16 significant digits).

TABLE 3

Comparison of the performance of the present method with QAWC in QUADPACK [17] *for* $⨍_0^1 \cos 2\pi at/(t-c)\,dt$, $a = 8, 16, 32$.

		$\varepsilon_a = 10^{-6}$				$\varepsilon_a = 10^{-10}$			
		present method		QUADPACK		present method		QUADPACK	
a	c	N	error	N	error	N	error	N	error
	0.6	⇑ (+1)	2×10^{-10}	325	2×10^{-11}	⇑ (+1)	1×10^{-13}	495	4×10^{-12}
8	0.8	**49**+1	1×10^{-10}	355	1×10^{-11}	**65**+1	1×10^{-13}	425	5×10^{-12}
	0.95	⇓ (+1)	3×10^{-11}	305	3×10^{-12}	⇓ (+1)	2×10^{-13}	505	4×10^{-12}
	0.6	⇑ (+1)	8×10^{-11}	555	2×10^{-11}	⇑ (+1)	6×10^{-13}	875	2×10^{-13}
16	0.8	**81**+1	1×10^{-10}	635	1×10^{-11}	**97**+1	5×10^{-14}	785	1×10^{-11}
	0.95	⇓ (+1)	5×10^{-12}	595	2×10^{-11}	⇓ (+1)	2×10^{-14}	975	2×10^{-12}
	0.6	⇑ (+1)	2×10^{-14}	1055	4×10^{-12}	⇑ (+1)	2×10^{-14}	1615	3×10^{-12}
32	0.8	**161**+1	9×10^{-14}	1205	5×10^{-12}	**161**+1	9×10^{-14}	1405	7×10^{-12}
	0.95	⇓ (+1)	7×10^{-14}	1125	3×10^{-11}	⇓ (+1)	7×10^{-14}	1595	8×10^{-13}

TABLE 4

Comparison of the performance of the present method with QAWC in QUADPACK [17] *for* $⨍_{-1}^1 (1-a^2)\ \ (1-2at+a^2)^{-1}\ /(t-c)\,dt$, $a = 0.8, 0.9, 0.95$.

		$\varepsilon_a = 10^{-6}$				$\varepsilon_a = 10^{-10}$			
		present method		QUADPACK		present method		QUADPACK	
a	c	N	error	N	error	N	error	N	error
	0.15	⇑ (+1)	4×10^{-9}	195	7×10^{-13}	⇑ (+1)	3×10^{-12}	305	3×10^{-13}
0.8	0.45	**97**+1	4×10^{-9}	205	1×10^{-12}	**129**+1	4×10^{-12}	305	4×10^{-13}
	0.95	⇓ (+1)	4×10^{-8}	305	2×10^{-12}	⇓ (+1)	1×10^{-11}	385	2×10^{-12}
	0.15	⇑ (+1)	4×10^{-8}	255	5×10^{-13}	⇑ (+1)	1×10^{-11}	365	3×10^{-13}
0.9	0.45	**193**+1	2×10^{-8}	265	9×10^{-13}	**257**+1	2×10^{-11}	375	4×10^{-13}
	0.95	⇓ (+1)	9×10^{-8}	335	2×10^{-12}	⇓ (+1)	1×10^{-10}	445	5×10^{-13}
	0.15	⇑ (+1)	6×10^{-9}	315	3×10^{-13}	⇑ (+1)	6×10^{-15}	425	2×10^{-13}
0.95	0.45	**385**+1	1×10^{-7}	325	6×10^{-13}	**641**+1	2×10^{-13}	435	3×10^{-13}
	0.95	⇓ (+1)	5×10^{-7}	395	2×10^{-12}	⇓ (+1)	8×10^{-13}	505	6×10^{-13}

TABLE 5

Comparison of the performance of the present method with QAWC in QUADPACK [17] *for* $⨍_0^1 \sqrt{1-t^2}\,/(t-c)\,dt$. *The number in the parentheses indicates failure to achieve the required accuracy.*

	$\varepsilon_a = 10^{-3}$				$\varepsilon_a = 10^{-5}$			
	present method		QUADPACK		present method		QUADPACK	
c	N	error	N	error	N	error	N	error
0.6	$\Uparrow^{(+1)}$	4×10^{-4}	(65)	2×10^{-3}	$\Uparrow^{(+1)}$	6×10^{-7}	315	3×10^{-9}
0.9	**97+1**	2×10^{-4}	285	3×10^{-7}	**1025+1**	6×10^{-6}	405	4×10^{-9}
0.95	$\Downarrow_{(+1)}$	1×10^{-4}	295	5×10^{-7}	$\Downarrow_{(+1)}$	7×10^{-6}	445	3×10^{-9}

APPENDIX A

Here, we prove (3.7). By using the relation

$$2\,T_n(t)\,T_m(t) = T_{n+m}(t) + T_{|n-m|}(t), \qquad n, m \geq 0, \tag{A.1}$$

and the definition of $\omega_{N+1}(t)$ (1.3) in (3.6), it follows that

$$\begin{aligned} 2\,\Omega_k^N(c) &= \int_{-1}^{1} \frac{\omega_{N+k+1}(t) - \omega_{N+k+1}(c)}{t-c}\,dt \\ &\pm \int_{-1}^{1} \frac{\omega_{|N-k|+1}(t) - \omega_{|N-k|+1}(c)}{t-c}\,dt, \qquad k \geq 0. \end{aligned} \tag{A.2}$$

In the above, the plus sign is taken if $N-k \geq 1$ and the minus sign if $k-N \geq 1$. Further, the second term in the right-hand side should be ignored when $k = N$.

Elliott [6] gives the identity involving the Chebyshev polynomial of the second kind $U_k(t)$:

$$T_{k+1}(t) - T_{k+1}(c) = 2\,(t-c) \sum_{n=0}^{k}{}' \, U_{k-n}(c)\,T_n(t), \qquad k \geq 0. \tag{A.3}$$

Using the identities $U_k(t) - U_{k-2}(t) = 2\,T_k(t)$ ($k \geq 1$), where we define $U_{-1}(t) = 0$, and (A.3) in (A.2) gives

$$\begin{aligned} \Omega_k^N(c) &= 2 \sum_{n=0}^{N+k}{}'' \, T_{N+k-n}(c) \int_{-1}^{1} T_n(t)\,dt \\ &\pm 2 \sum_{n=0}^{|N-k|}{}'' \, T_{|N-k|-n}(c) \int_{-1}^{1} T_n(t)\,dt. \end{aligned} \tag{A.4}$$

Thus, $\Omega_k^N(c)$ is bounded by

$$|\Omega_k^N(c)| \leq 2 \sum_{n=0}^{N+k}{}'' \left| \int_{-1}^{1} T_n(t)\,dt \right| + 2 \sum_{n=0}^{|N-k|}{}'' \left| \int_{-1}^{1} T_n(t)\,dt \right|. \tag{A.5}$$

If one notes in (A.5) that the integral $\int_{-1}^{1} T_n(t)\,dt$ equals $2/(1-n^2)$ if n is even, and vanishes otherwise, it is easy to verify (3.7).

Acknowledgment

We are indebted to H. Sugiura for helpful comments.

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