CLENSHAW–CURTIS AND GAUSS–LEGENDRE QUADRATURE FOR CERTAIN BOUNDARY ELEMENT INTEGRALS*

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Abstract. Following a recent article by Trefethen [*SIAM Review*, 50 (2008), pp. 67–87], the use of Clenshaw–Curtis quadrature rather than Gauss–Legendre quadrature for nearly singular integrals which arise in the boundary element method has been investigated. When these quadrature rules are used in association with the sinh-transformation, the authors have concluded, after considering asymptotic estimates of the truncation errors for certain proto-type functions arising in this context, that Gauss–Legendre quadrature should continue to be the preferred quadrature rule.

Key words. Clenshaw–Curtis quadrature, Gauss–Legendre quadrature, boundary element integrals

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1. Introduction. Recently, in an excellent article, Trefethen [9] has considered the relationship between Clenshaw–Curtis (CC) and Gauss–Legendre (GL) quadrature for integrals of the form $\int_{-1}^1 f(x) dx$. One of Trefethen’s conclusions is that if f is analytic in a small neighborhood of $[-1, 1]$, then the two quadrature formulas should have about the same accuracy. In the boundary element method we have exactly this situation when dealing with nearly singular integrals. In [5], [6], and [7] the authors have used Gauss–Legendre quadrature in association with the so-called “sinh-transformation”. The purpose of this paper is to investigate whether Gauss–Legendre quadrature should be replaced by Clenshaw–Curtis quadrature in this particular context. One advantage of the latter over the former is that far less computation is required to generate the quadrature rule; that is, to calculate its weights and nodes.

We shall consider this question by obtaining realistic truncation error estimates for both quadrature rules and for three prototype integrals which arise in the boundary element method. For $j = 1, 2, 3$ we shall consider the integrals

$$(1.1) \quad I_j := \int_{-1}^1 f_j(x) dx$$

where

$$(1.2) \quad f_1(x) := x^k / ((x - a)^2 + b^2),$$

$$(1.3) \quad f_2(x) := x^k \log((x - a)^2 + b^2),$$

and

$$(1.4) \quad f_3(x) := x^k ((x - a)^2 + b^2)^\lambda.$$

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In each of these we shall assume that

$$(1.5) \quad -1 < a < 1, \quad 0 < b \ll 1,$$

and that k is a small nonnegative integer which allows for the various types of basis functions arising in the boundary element method; see, for example, Brebbia and Dominguez [2].

In (1.4), λ is a noninteger > -1 and is of particular interest in the boundary element method when $\lambda = -1/2$. From (1.2) to (1.4) we see that in each case the function f_j , when its definition is continued into the complex z -plane, where $z = x + iy$, has singularities at the points z_0 and $\bar{z}_0$ where

$$(1.6) \quad z_0 := a + ib.$$

Under the conditions of (1.5) these singularities can be considered as “close” to the interval of integration.

In order to obtain expressions for the truncation errors of the quadrature rules, we shall use the theory given by Donaldson and Elliott [3] to obtain *asymptotic* estimates for n large, where n is the number of quadrature points. Experience has shown that even with this assumption, the error estimates give one or two correct significant figures even for moderate values of n . If $E_n f$ denotes the truncation error for an n -point quadrature rule, then, from [3], we can write

$$(1.7) \quad E_n f = \frac{1}{2\pi i} \int_C f(z) k_n(z) dz,$$

where C is a contour, containing the interval $(-1, 1)$, on and within which f is analytic. The function k_n , which depends only on the quadrature rule, is analytic in the z -plane with the interval $[-1, 1]$ deleted and, for n -point interpolatory quadrature, will tend to zero at least like $O(|z|^{-n})$, as $|z|$ tends to infinity. Because of this, we can deform the contour C away from the interval $[-1, 1]$, but in such a way that the singularities at z_0 and $\bar{z}_0$ are avoided and f continues to be analytic on and within C . In Figure 2.1 we have shown the contour C when f has branch points at z_0 and $\bar{z}_0$. Since $|k_n(z)| \rightarrow 0$ as $|z| \rightarrow \infty$ we have that if, for the function f_1 we have $k < n + 1$, for the function f_2 , $k < n - 2$ and, for the function f_3 , that $k + 2\lambda < n - 1$, then the contribution to $E_n f$ from those parts of the contour C which are well removed from the interval $[-1, 1]$ will tend to zero. The error $E_n f$ will be given by the contributions from the simple poles at $z_0, \bar{z}_0$ in the case of f_1 , or from the integrals along the branch cuts from z_0 to ∞ and $\bar{z}_0$ to ∞ for the functions f_2 and f_3 .

In section 2 we shall obtain the generic forms of $E_n f$ for each of f_1, f_2 , and f_3 . In section 3 we shall consider explicitly the asymptotic forms of $E_n^{GL} f$ for n -point Gauss-Legendre quadrature and see how these estimates compare with the actual truncation errors in certain cases. In section 4, we shall consider $(n + 1)$ -point Clenshaw-Curtis quadrature where the $n + 1$ points are chosen as the extrema of the Chebyshev polynomial of the first kind, T_n . These are the points $x_{j,n} = \cos(\pi j/n), j = 0(1)n$. We shall compare our asymptotic estimates for $E_{n+1}^{CC} f$ with the actual errors only when n is even.

It is of necessity that the analysis of the truncation errors to be given in sections 2-4 is rather technical. For the reader who does not wish to plough through this analysis, may we suggest that the numerical results in Tables 3.1 to 3.3 and 4.1 to 4.3 be studied. These examples indicate that one can have some faith in the asymptotic error estimates that have been derived and from which the important conclusions given in section 5 are based.

FIG. 2.1.

2. Asymptotic error estimates for the functions f_1 , f_2 , and f_3 . Let us first consider the function f_1 where, see (1.2) and (1.6),

$$(2.1) \quad f_1(z) = \frac{z^k}{(z-a)^2 + b^2} = \frac{z^k}{(z-z_0)(z-\bar{z}_0)}.$$

Then, from (1.7),

$$(2.2) \quad E_n f_1 = \frac{1}{2\pi i} \int_C \frac{z^k k_n(z)}{(z-z_0)(z-\bar{z}_0)} dz,$$

where C is a contour, containing the interval $(-1, 1)$, on and within which f_1 is analytic. Now the function f_1 has simple poles at z_0 and $\bar{z}_0$ with residues given by $z_0^k/(z_0 - \bar{z}_0)$ and $\bar{z}_0^k/(\bar{z}_0 - z_0)$, respectively. If we let C tend to infinity then, provided $k < n + 1$, we have simply that

$$(2.3) \quad E_n f_1 = -\frac{1}{b} \Im(z_0^k k_n(z_0)).$$

This will be the starting point, in section 3 and section 4, respectively, for estimating $E_n^{GL} f_1$ and $E_{n+1}^{CC} f_1$.

Consider now the function f_2 where, from (1.3) and (1.6), we have

$$(2.4) \quad f_2(z) = z^k \log((z-a)^2 + b^2) = z^k \log(z-z_0) + z^k \log(z-\bar{z}_0).$$

Thus we may write

$$(2.5) \quad E_n f_2 = E_n f_2(z_0) + E_n f_2(\bar{z}_0),$$

where

$$(2.6) \quad E_n f_2(z_0) := \frac{1}{2\pi i} \int_{C_1} z^k k_n(z) \log(z - z_0) dz$$

and

$$(2.7) \quad E_n f_2(\bar{z}_0) := \frac{1}{2\pi i} \int_{C_2} z^k k_n(z) \log(z - \bar{z}_0) dz.$$

Here C_1 is the contour of Figure 2.1 without the branch cut from $\bar{z}_0$ to ∞ and C_2 is the contour of Figure 2.1 without the branch cut from z_0 to ∞ . In (2.6), the function $\log(z - z_0)$ has a branch point at z_0 , and we shall define a branch cut $B_{(z_0)}$ from z_0 to infinity, which does not cross $[-1, 1]$, by writing

$$(2.8) \quad B_{(z_0)} = \left\{ z(s) \in \mathbf{C} : z(s) = \frac{1}{2} \left(\xi_0 s + \frac{1}{\xi_0 s} \right), \quad 1 \leq s < \infty \right\},$$

where

$$(2.9) \quad \xi_0 := z_0 + \sqrt{z_0^2 - 1}.$$

The function $\sqrt{z_0^2 - 1}$ is defined as $\sqrt{z_0 - 1}\sqrt{z_0 + 1}$ with $-\pi < \arg(z_0 \pm 1) \leq \pi$. Consequently, ξ_0 is such that $|\xi_0| = \rho > 1$. We see from (2.8) that with $s = 1$ we have $z(1) = z_0$ since, from (2.9), $1/\xi_0 = z_0 - \sqrt{z_0^2 - 1}$. Again it is not difficult to show that $B_{(z_0)}$ is the arc of a hyperbola. For if we write $\xi_0 = \rho e^{i\phi}$, then from (2.8), on writing $z(s) = x(s) + iy(s)$, we have

$$(2.10) \quad x(s) = \frac{1}{2} \left(\rho s + \frac{1}{\rho s} \right) \cos \phi, \quad y(s) = \frac{1}{2} \left(\rho s - \frac{1}{\rho s} \right) \sin \phi.$$

Provided ϕ is not an integer multiple of $\pi/2$, it follows that

$$(2.11) \quad \frac{x^2}{\cos^2 \phi} - \frac{y^2}{\sin^2 \phi} = 1,$$

which is a hyperbola with foci at the points $(\pm 1, 0)$.

We shall define $\log(z - z_0)$ along the lower side of the branch cut $B_{(z_0)}$ and will exclude the upper side. In order to evaluate $E_n f_2(z_0)$ we shall let the contour C_1 tend to infinity. Then, provided $k < n - 1$, we shall have

$$(2.12) \quad E_n f_2(z_0) = \frac{1}{2\pi i} \int_{AB \cup CD} z^k k_n(z) \log(z - z_0) dz.$$

Since along $B_{(z_0)}$ we have $z = z(s)$ with $1 \leq s < \infty$ (see (2.8)) we have

$$(2.13) \quad E_n f_2(z_0) = \frac{1}{2\pi i} \int_1^\infty z^k(s) k_n(z(s)) [\log(z(s) - z_0)|_{CD} - \log(z(s) - z_0)|_{AB}] z'(s) ds,$$

where $\log(z(s) - z_0)|_{AB}$ is the value of the log function along AB and $\log(z(s) - z_0)|_{CD}$ is the value of the log function along the upper side CD of the cut $B_{(z_0)}$. We have

$$(2.14) \quad (z(s) - z_0)|_{CD} = (z(s) - z_0)|_{AB} e^{-2\pi i}$$

so that

$$(2.15) \quad \log(z(s) - z_0)|_{CD} - \log(z(s) - z_0)|_{AB} = -2\pi i$$

and from (2.13) we find

$$(2.16) \quad E_n f_2(z_0) = - \int_1^\infty z^k(s) k_n(z(s)) z'(s) ds.$$

It is not difficult to show that $E_n f_2(\bar{z}_0) = \overline{E_n f_2(z_0)}$ so that from (2.5) and (2.16) we have

$$(2.17) \quad E_n f_2 = -2\Re \left(\int_1^\infty z^k(s) k_n(z(s)) z'(s) ds \right).$$

Since, from (2.8),

$$(2.18) \quad z'(s) = \frac{\xi_0}{2} \left(1 - \frac{1}{\xi_0^2 s^2} \right)$$

and since,

$$(2.19) \quad z^k(s) = \frac{1}{2^k} \sum_{l=0}^k \binom{k}{l} \xi_0^{k-2l} s^{k-2l},$$

it follows that

$$(2.20) \quad E_n f_2 = -\frac{1}{2^k} \sum_{l=0}^k \binom{k}{l} \Re \left(\xi_0^{k-2l+1} \int_1^\infty s^{k-2l} k_n(z(s)) \left(1 - \frac{1}{\xi_0^2 s^2} \right) ds \right).$$

We shall take (2.20) as our starting point, in section 3 and section 4, respectively, for estimating $E_n^{GL} f_2$ and $E_{n+1}^{CC} f_2$.

Finally, let us consider the function f_3 as defined in (1.4). Arguing as before we find

$$(2.21) \quad E_n f_3 = \frac{1}{2\pi i} \int_C z^k k_n(z) (z - z_0)^\lambda (z - \bar{z}_0)^\lambda dz,$$

where the contour C is initially chosen so that $(z - z_0)^\lambda (z - \bar{z}_0)^\lambda$ is analytic on and within C . In order to evaluate $E_n f_3$ we shall consider separately the contributions from the neighborhoods of z_0 and $\bar{z}_0$. If $E_n f_3(z_0)$ denotes the contribution from the neighborhood of z_0 , then from (2.21) we have approximately that

$$(2.22) \quad E_n f_3(z_0) = (z_0 - \bar{z}_0)^\lambda J_1(z_0) = (2b)^\lambda e^{i\pi\lambda/2} J_1(z_0)$$

where

$$(2.23) \quad J_1(z_0) := \frac{1}{2\pi i} \int_{C_1} z^k k_n(z) (z - z_0)^\lambda dz.$$

Similarly we have

$$(2.24) \quad E_n f_3(\bar{z}_0) = (\bar{z}_0 - z_0)^\lambda J_2(\bar{z}_0) = (2b)^\lambda e^{-i\pi\lambda/2} J_2(\bar{z}_0),$$

where

$$(2.25) \quad J_2(\bar{z}_0) := \frac{1}{2\pi i} \int_{C_2} z^k k_n(z) (z - \bar{z}_0)^\lambda dz.$$

The contours C_1 and C_2 are as described for equations (2.6) and (2.7), respectively. From (2.21)–(2.25) we have

$$(2.26) \quad E_n f_3 = (2b)^\lambda [e^{i\pi\lambda/2} J_1(z_0) + e^{-i\pi\lambda/2} J_2(\bar{z}_0)],$$

approximately. Let us consider the evaluation of $J_1(z_0)$. For the function $(z - z_0)^\lambda$ we shall assume, as we did for $\log(z - z_0)$, that it is defined on the lower side of the cut $B(z_0)$, i.e., along AB . Then we have, from (2.14),

$$(2.27) \quad (z(s) - z_0)^\lambda|_{CD} = (z(s) - z_0)^\lambda|_{AB} e^{-2\pi i\lambda}.$$

From (2.23), since $B(z_0)$ is defined by (2.8), then if we also assume that $k + 2\lambda < n - 1$, we find

$$\begin{aligned} J_1(z_0) &= \frac{1}{2\pi i} \int_{AB \cup CD} z^k k_n(z) (z - z_0)^\lambda dz \\ &= \frac{1}{2\pi i} \int_1^\infty z^k(s) k_n(z(s)) [(z(s) - z_0)^\lambda|_{CD} - (z(s) - z_0)^\lambda|_{AB}] z'(s) ds \\ (2.28) \quad &= \frac{(e^{-2\pi i\lambda} - 1)}{2\pi i} \int_1^\infty z^k(s) k_n(z(s)) (z(s) - z_0)^\lambda z'(s) ds. \end{aligned}$$

From this and (2.22) we obtain

$$(2.29) \quad E_n f_3(z_0) = -\frac{(2b)^\lambda \sin(\pi\lambda) e^{-i\pi\lambda/2}}{\pi} \int_1^\infty (z(s) - z_0)^\lambda z^k(s) k_n(z(s)) z'(s) ds.$$

We may proceed similarly to evaluate $E_n f_3(\bar{z}_0)$, and we shall find that $E_n f_3(\bar{z}_0) = \overline{E_n f_3(z_0)}$ so that, since $E_n f_3 = E_n f_3(z_0) + E_n f_3(\bar{z}_0)$, we have

$$(2.30) \quad E_n f_3 = -\frac{2^{1+\lambda} b^\lambda \sin(\pi\lambda)}{\pi} \Re \left(e^{-i\pi\lambda/2} \int_1^\infty z^k(s) k_n(z(s)) (z(s) - z_0)^\lambda z'(s) ds \right),$$

approximately. Since $z_0 = z(1)$ it follows from (2.8) that

$$(2.31) \quad (z(s) - z_0)^\lambda = \frac{(s-1)^\lambda \xi_0^\lambda}{2^\lambda} \left(1 - \frac{1}{\xi_0^2 s} \right)^\lambda.$$

Again, on using (2.18) and (2.19) we obtain from (2.30) that

$$\begin{aligned} (2.32) \quad E_n f_3 &= -\frac{b^\lambda \sin(\pi\lambda)}{2^k \pi} \Re \left(e^{-i\pi\lambda/2} \sum_{l=0}^k \binom{k}{l} \xi_0^{k-2l+\lambda+1} \right. \\ &\quad \times \left. \int_1^\infty s^{k-2l} (s-1)^\lambda \left(1 - \frac{1}{\xi_0^2 s} \right)^\lambda \left(1 - \frac{1}{\xi_0^2 s^2} \right) k_n(z(s)) ds \right). \end{aligned}$$

This is the required generic form for $E_n f_3$. Let us now consider the asymptotic truncation error estimates for Gauss–Legendre quadrature.

TABLE 3.1
 f_1 with $a = 0.5$, $k = 2$, $n = 30$, Gauss–Legendre quadrature.

b	Actual GL error	Asymptotic estimate (3.4)
0.05	0.726	0.735
0.10	0.113×10^{-1}	0.113×10^{-1}
0.15	0.268×10^{-3}	0.268×10^{-3}
0.20	0.806×10^{-5}	0.802×10^{-5}

3. Gauss–Legendre quadrature. Consider n -point Gauss–Legendre quadrature. We shall use the symbol $\sim$ to mean “asymptotically equal to.” That is, $a(n) \sim b(n)$, for large n , if $\lim_{n \rightarrow \infty} a(n)/b(n) = 1$. Donaldson and Elliott [3] have shown in this case that, for $z \in \mathbf{C} \setminus [-1, 1]$ and n large,

$$(3.1) \quad k_n^{GL}(z) \sim \frac{c_n}{(z + \sqrt{z^2 - 1})^{2n+1}},$$

where

$$(3.2) \quad c_n := \frac{2\pi(\Gamma(n+1))^2}{\Gamma(n+1/2)\Gamma(n+3/2)}.$$

For the function f_1 the truncation error $E_n^{GL} f_1$ is given, from (2.3) and (3.1), as

$$(3.3) \quad E_n^{GL} f_1 \sim -\frac{c_n}{b} \Im \left(\frac{z_0^k}{(z_0 + \sqrt{z_0^2 - 1})^{2n+1}} \right),$$

for large n . Since, from (2.8), $z_0 = z(1)$, then, from (2.19) with $s = 1$, and (3.3) we obtain

$$(3.4) \quad E_n^{GL} f_1 \sim -\frac{c_n}{2^k b} \sum_{l=0}^k \binom{k}{l} \Im \left(\frac{1}{\xi_0^{2n+1+2l-k}} \right).$$

For a particular example, let us consider the case where $f_1(x) = x^2/((x-a)^2 + b^2)$ so that $k = 2$. We then have

$$(3.5) \quad I_1 = \int_{-1}^1 f_1(x) dx = 2 + a \ln \left(\frac{(1-a)^2 + b^2}{(1+a)^2 + b^2} \right) + \frac{(a^2 - b^2)}{b} \left(\arctan \left(\frac{1+a}{b} \right) + \arctan \left(\frac{1-a}{b} \right) \right).$$

In Table 3.1 we give the actual errors in Gauss–Legendre quadrature for the case when $n = 30$, $a = 0.5$, and $b = 0.05(0.05)0.20$. We also present the asymptotic estimates as given by (3.4). As can be seen, for this example the agreement between the actual errors for 30-point Gauss–Legendre quadrature and the asymptotic estimates is excellent.

Now consider the function f_2 . We first observe from (2.8) that if we define

$$(3.6) \quad \xi(s) := z(s) + \sqrt{z(s)^2 - 1},$$

then

$$(3.7) \quad \xi(s) = \xi_0 s, \quad 1 \leq s < \infty,$$

TABLE 3.2
 f_2 with $a = -0.25$, $k = 1$, $n = 20$, Gauss-Legendre quadrature.

b	Actual GL error	Asymptotic estimate (3.8)
0.05	-0.316×10^{-2}	-0.346×10^{-2}
0.10	-0.312×10^{-3}	-0.318×10^{-3}
0.15	-0.322×10^{-4}	-0.324×10^{-4}
0.20	-0.412×10^{-5}	-0.415×10^{-5}

on recalling the definition of ξ_0 in (2.9). From (2.17), (2.18), (2.19), (3.1), and (3.7) we find

$$\begin{aligned}
 E_n^{GL} f_2 &\sim -\frac{c_n}{2^k} \sum_{l=0}^k \binom{k}{l} \Re \left(\frac{1}{\xi_0^{2n+2l-k}} \left(\int_1^\infty s^{-2n-2l+k-1} ds - \frac{1}{\xi_0^2} \int_1^\infty s^{-2n-2l+k-3} ds \right) \right) \\
 (3.8) \quad &= -\frac{c_n}{2^k} \sum_{l=0}^k \binom{k}{l} \Re \left(\frac{1}{\xi_0^{2n+2l-k}} \left(\frac{1}{(2n+2l-k)} - \frac{1}{\xi_0^2(2n+2l-k+2)} \right) \right).
 \end{aligned}$$

Consider the integral I_2 where

$$\begin{aligned}
 (3.9) \quad I_2 &= \int_{-1}^1 x \log((x-a)^2 + b^2) dx = -2a + \frac{(1-a^2+b^2)}{2} \log \left(\frac{(1-a)^2 + b^2}{(1+a)^2 + b^2} \right) \\
 &\quad + 2ab \left(\arctan \left(\frac{1-a}{b} \right) + \arctan \left(\frac{1+a}{b} \right) \right),
 \end{aligned}$$

so that we are choosing f_2 of (1.3) with $k = 1$. In Table 3.2 we compare the actual quadrature error with the asymptotic estimate given by (3.8), for the particular case when $n = 20$, $a = -0.25$, and $b = 0.05(0.05)0.20$. Again, we see that the asymptotic estimates, obtained under the assumption that n is large, agree well with the actual errors even when $n = 20$.

Finally, let us consider the function f_3 . From (2.18), (2.32), (3.1), (3.6), and (3.7) we first of all find that, for large n ,

$$\begin{aligned}
 (3.10) \quad E_n^{GL} f_3 &\sim -\frac{c_n b^\lambda \sin(\pi\lambda)}{\pi 2^k} \sum_{l=0}^k \binom{k}{l} \\
 &\quad \times \Re \left(\frac{e^{-i\pi\lambda/2}}{\xi_0^{2n+2l-k-\lambda}} \left(\int_1^\infty s^{-2n-2l+k-1} (s-1)^\lambda \left(1 - \frac{1}{\xi_0^2 s} \right)^\lambda ds \right. \right. \\
 &\quad \left. \left. - \frac{1}{\xi_0^2} \int_1^\infty s^{-2n-2l+k-3} (s-1)^\lambda \left(1 - \frac{1}{\xi_0^2 s} \right)^\lambda ds \right) \right).
 \end{aligned}$$

In each integral we observe, since we are assuming that n is large, that the major contribution to the integral comes from the neighborhood of $s = 1$. On replacing $(1 - 1/(\xi_0^2 s))^\lambda$ by $(1 - 1/\xi_0^2)^\lambda$ we obtain

$$\begin{aligned}
 (3.11) \quad E_n^{GL} f_3 &\sim -\frac{c_n b^\lambda \sin(\pi\lambda)}{\pi 2^k} \sum_{l=0}^k \binom{k}{l} \Re \left(\frac{e^{-i\pi\lambda/2}}{\xi_0^{2n+2l-k-\lambda}} \left(1 - \frac{1}{\xi_0^2} \right)^\lambda \left(J(n) - \frac{1}{\xi_0^2} J(n+1) \right) \right),
 \end{aligned}$$

say, where

$$(3.12) \quad J(n) := \int_1^\infty s^{-2n-2l+k-1} (s-1)^\lambda ds.$$

On putting $s = 1/t$ we find

$$(3.13) \quad J(n) = \int_0^1 t^{2n+2l-k-\lambda-1} (1-t)^\lambda dt = \frac{\Gamma(2n+2l-k-\lambda)\Gamma(1+\lambda)}{\Gamma(2n+2l-k+1)},$$

from Abramowitz and Stegun [1, sections 6.2.1 and 6.2.2]. Since we are assuming that n is large we have, from Abramowitz and Stegun [1, section 6.1.47], that

$$(3.14) \quad \frac{\Gamma(2n+2l-k-\lambda)}{\Gamma(2n+2l-k+1)} \sim \frac{1}{(2n)^{1+\lambda}}$$

so that we find

$$(3.15) \quad J(n) \sim \frac{\Gamma(1+\lambda)}{(2n)^{1+\lambda}}.$$

Substituting this into (3.11) gives

$$(3.16) \quad \begin{aligned} E_n^{GL} f_3 &\sim -\frac{c_n b^\lambda \sin(\pi\lambda)\Gamma(1+\lambda)}{\pi 2^k} \sum_{l=0}^k \binom{k}{l} \Re \\ &\quad \times \left(\frac{e^{-i\pi\lambda/2}}{\xi_0^{2n+2l-k-\lambda}} \left(1 - \frac{1}{\xi_0^2}\right)^\lambda \left(\frac{1}{(2n)^{1+\lambda}} - \frac{1}{(2n+2)^{1+\lambda}\xi_0^2} \right) \right) \\ &= -\frac{c_n b^\lambda \sin(\pi\lambda)\Gamma(1+\lambda)}{\pi 2^{k+1+\lambda} n^{1+\lambda}} \sum_{l=0}^k \binom{k}{l} \Re \left(\frac{e^{-i\pi\lambda/2}}{\xi_0^{2n+2l-k-\lambda}} \left(1 - \frac{1}{\xi_0^2}\right)^{1+\lambda} \right) \end{aligned}$$

for large n .

Let us consider a particular example. If we choose, in (1.4), $k = 0$ and $\lambda = -1/2$, then we have simply

$$(3.17) \quad I_3 = \int_{-1}^1 f_3(x) dx = \operatorname{arcsinh}\left(\frac{1-a}{b}\right) + \operatorname{arcsinh}\left(\frac{1+a}{b}\right).$$

With $k = 0$ and $\lambda = -1/2$ in the asymptotic error estimate (3.16) we find

$$(3.18) \quad E_n^{GL} f_3 \sim \frac{c_n}{\sqrt{2\pi b n}} \Re \left(\frac{e^{i\pi/4}}{\xi_0^{2n+1/2}} \left(1 - \frac{1}{\xi_0^2}\right)^{1/2} \right).$$

In Table 3.3 we have compared the actual truncation error with this asymptotic estimate for the case when $n = 30$, $a = 0.75$, and $b = 0.05(0.05)0.30$. Once again the agreement between the asymptotic estimate of $E_n^{GL} f_3$ and the actual truncation error is excellent. So much for Gauss–Legendre quadrature. In the next section we shall give a similar analysis for Clenshaw–Curtis quadrature.

TABLE 3.3
 f_3 with $a = 0.75$, $\lambda = -0.5$, $k = 0$, $n = 30$, Gauss–Legendre quadrature.

b	Actual GL error	Asymptotic estimate (3.18)
0.05	$+0.781 \times 10^{-2}$	$+0.798 \times 10^{-2}$
0.10	$+0.154 \times 10^{-3}$	$+0.157 \times 10^{-3}$
0.15	$+0.218 \times 10^{-5}$	$+0.220 \times 10^{-5}$
0.20	$+0.899 \times 10^{-8}$	$+0.893 \times 10^{-8}$
0.25	-0.604×10^{-9}	-0.610×10^{-9}
0.30	-0.162×10^{-10}	-0.163×10^{-10}

4. Clenshaw–Curtis quadrature. By Clenshaw–Curtis quadrature we shall mean the particular quadrature rule obtained by integration of the Lagrange interpolation polynomial of degree n which takes the value of the function at the $n+1$ points $x_{j,n}$, $j = 0(1)n$, defined by

$$(4.1) \quad x_{j,n} = \cos(\pi j/n).$$

Trefethen [9] calls these the “Chebyshev points” and they are the zeros of the polynomial $(z^2 - 1)U_{n-1}(z)$, where U_{n-1} denotes the Chebyshev polynomial of the second kind of degree $n-1$; see, for example, Mason and Handscomb [8]. Since we are going to represent the truncation error in the Clenshaw–Curtis quadrature rule as a contour integral, recall (1.7), our first task is to find the function, let us call it k_{n+1}^{CC} , so that

$$(4.2) \quad E_{n+1}^{CC} f = \frac{1}{2\pi i} \int_C f(z) k_{n+1}^{CC}(z) dz.$$

Let us note here that essentially what we are proposing to do is to compare this $(n+1)$ -point Clenshaw–Curtis quadrature rule with the n -point Gauss–Legendre rule of the previous section.

From Donaldson and Elliott [3, Table 1] we have

$$(4.3) \quad k_{n+1}^{CC}(z) = \frac{1}{(z^2 - 1)U_{n-1}(z)} \int_{-1}^1 \frac{(t^2 - 1)U_{n-1}(t)}{z - t} dt,$$

for $z \in \mathbf{C} \setminus [-1, 1]$. Let us define

$$(4.4) \quad J(n; z_0) := \int_{-1}^1 \frac{(t^2 - 1)U_{n-1}(t)}{z_0 - t} dt$$

for $z_0 \in \mathbf{C} \setminus [-1, 1]$, and rewrite it as

$$(4.5) \quad J(n; z_0) = - \int_{-1}^1 \sqrt{1 - t^2} g(t; z_0) U_{n-1}(t) dt$$

where

$$(4.6) \quad g(t; z_0) := \frac{\sqrt{1 - t^2}}{z_0 - t}, \quad -1 \leq t \leq 1.$$

Suppose we can write

$$(4.7) \quad g(t; z_0) = \sum_{k=0}^{\infty} b_k(z_0) U_k(t).$$

On substituting this back into (4.5) and recalling that

$$(4.8) \quad \int_{-1}^1 \sqrt{1-t^2} U_k(t) U_{n-1}(t) dt = \frac{\pi}{2} \delta_{k,n-1},$$

we have at once that

$$(4.9) \quad J(n; z_0) = -\frac{\pi}{2} b_{n-1}(z_0),$$

so that the problem becomes one of estimating $b_{n-1}(z_0)$ under the assumption that n is large. Following Elliott [4] we can express $b_{n-1}(z_0)$ as a contour integral. Suppose, for some general function f , that

$$(4.10) \quad f(x) = \sum_{k=0}^{\infty} a_k U_k(x)$$

for $-1 \leq x \leq 1$, and that the definition of f can be extended from $(-1, 1)$ into the complex z -plane. Using Cauchy's integral formula, it can be shown, following [4], that

$$(4.11) \quad a_k = \frac{1}{\pi i} \int_C \frac{f(z)}{(z + \sqrt{z^2 - 1})^{k+1}} dz,$$

$k \in \mathbf{N}_0$, where C is a contour enclosing $(-1, 1)$, on and within which f is analytic. Returning to our specific problem, we extend the definition of g as given in (4.6) into the z -plane by writing

$$(4.12) \quad g(z; z_0) = \frac{\sqrt{1-z}\sqrt{1+z}}{z_0 - z}.$$

Here $\sqrt{1-z}$ is defined in the plane cut along the positive real axis from $+1$ to $+\infty$ so that $-\pi < \arg(1-z) \leq \pi$. As before, $\sqrt{1+z} = \sqrt{z+1}$ with $-\pi < \arg(1+z) \leq \pi$. We observe that unlike the function $\sqrt{z^2-1}$, the function $\sqrt{1-z^2}$ is defined for $-1 < \Re z < 1$. This distinction between $\sqrt{1-z^2}$ and $\sqrt{z^2-1}$ must be preserved throughout.

Consider now the evaluation of $b_{n-1}(z_0)$ where we shall assume that z_0 is not real. We have from (4.7), (4.11), and (4.12) that

$$(4.13) \quad b_{n-1}(z_0) = \frac{1}{\pi i} \int_C \frac{g(z; z_0)}{(z + \sqrt{z^2 - 1})^n} dz.$$

In order to evaluate this contour integral, let us deform C as shown in Figure 4.1. Let $\mathcal{E}_\rho$ denote the ellipse $|z + \sqrt{z^2 - 1}| = \rho > 1$ which has foci at $(+1, 0)$ and $(-1, 0)$ and semi-major and minor axes given by $(\rho + 1/\rho)/2$ and $(\rho - 1/\rho)/2$, respectively. As we let $\rho \rightarrow \infty$, the integral over $\mathcal{E}_\rho$ tends to zero. Since the function $g(z; z_0)$ has a simple pole at z_0 , we find

$$(4.14) \quad b_{n-1}(z_0) = \frac{2\sqrt{1-z_0^2}}{(z_0 + \sqrt{z_0^2 - 1})^n} + b_{n-1}^{(1)}(z_0) + b_{n-1}^{(2)}(z_0),$$

where we define

$$(4.15) \quad b_{n-1}^{(1)}(z_0) := \frac{1}{\pi i} \int_{AB \cup CD} \frac{g(z; z_0)}{(z + \sqrt{z^2 - 1})^n} dz$$

FIG. 4.1.

and

$$(4.16) \quad b_{n-1}^{(2)}(z_0) := \frac{1}{\pi i} \int_{EF \cup GH} \frac{g(z; z_0)}{(z + \sqrt{z^2 - 1})^n} dz.$$

Consider first the evaluation of $b_{n-1}^{(1)}(z_0)$. Let $B_{(1)}$ denote the branch cut from $+1$ to $+\infty$ along the positive real axis. If $z(s)$ denotes a point on $B_{(1)}$, then we may write

$$(4.17) \quad z(s) = \frac{1}{2} \left(s + \frac{1}{s} \right) \quad \text{for } 1 \leq s < \infty.$$

(We choose this rather than simply $z = s$, $1 \leq s < \infty$ since this parameterization is a special case of (2.8) and, as we have seen, gives rise to integrals that are readily evaluated.) From (4.17) we have

$$(4.18) \quad \sqrt{z^2(s) - 1} = \frac{1}{2} \left(s - \frac{1}{s} \right)$$

so that we have simply

$$(4.19) \quad z(s) + \sqrt{z^2(s) - 1} = s.$$

Finally we note that

$$(4.20) \quad z'(s) = \frac{1}{2} \left(1 - \frac{1}{s^2} \right).$$

From (4.12), (4.15), (4.17), (4.19), and (4.20) we find

$$(4.21) \quad b_{n-1}^{(1)}(z_0) = \frac{1}{2\pi i} \int_1^\infty \frac{(1 - 1/s^2)}{s^n(z_0 - (s + 1/s)/2)} \left(\sqrt{1 - z^2(s)}|_{CD} - \sqrt{1 - z^2(s)}|_{AB} \right) ds,$$

where $\sqrt{1-z^2(s)}|_{CD}$ denotes the value of that function along CD . Now

$$(4.22) \quad \sqrt{1-z^2(s)}|_{CD} = \sqrt{1-z^2(s)}|_{AB} e^{-i\pi},$$

and, furthermore, along AB we have

$$(4.23) \quad \sqrt{1-z^2(s)}|_{AB} = \frac{s}{2} \left(1 - \frac{1}{s^2}\right) e^{i\pi/2}.$$

From (4.21)–(4.23) we obtain

$$(4.24) \quad b_{n-1}^{(1)}(z_0) = -\frac{1}{2\pi} \int_1^\infty \frac{(1-1/s^2)^2}{s^{n-1}(z_0 - (s+1/s)/2)} ds.$$

Since we are assuming $n \gg 1$, we see that the major contribution to the integrand comes from the neighborhood of $s = 1$ so that on replacing $(z_0 - (s+1/s)/2)$ by $(z_0 - 1)$ and also, after evaluating the resulting integral, $n(n^2 - 4)$ by n^3 we find that

$$(4.25) \quad b_{n-1}^{(1)}(z_0) \sim -\frac{4}{\pi n^3(z_0 - 1)}.$$

We may proceed similarly for $b_{n-1}^{(2)}(z_0)$ by writing

$$(4.26) \quad z(s) = -(s+1/s)/2, \quad \text{for } 1 \leq s < \infty.$$

Omitting the details we find

$$(4.27) \quad b_{n-1}^{(2)}(z_0) \sim \frac{4(-1)^n}{\pi n^3(z_0 + 1)}.$$

From (4.9), (4.14), (4.25), and (4.27) we obtain

$$(4.28) \quad J(n; z_0) \sim -\frac{\pi\sqrt{1-z_0^2}}{(z_0 + \sqrt{z_0^2-1})^n} - \frac{2}{n^3} \left(\frac{(-1)^n}{z_0+1} - \frac{1}{z_0-1} \right),$$

assuming that $n \gg 1$. Finally, we are in a position to give an appropriate expression for $k_{n+1}^{CC}(z)$; see (4.3). On recalling that for $z \in \mathbf{C}$ we have

$$(4.29) \quad U_{n-1}(z) = \frac{1}{2\sqrt{z^2-1}} \left((z + \sqrt{z^2-1})^n - (z - \sqrt{z^2-1})^n \right),$$

see Mason and Handscomb [8, (1.52)], we find from (4.3), (4.4), (4.28), and (4.29) that for $z \in \mathbf{C} \setminus [-1, 1]$,

$$(4.30) \quad k_{n+1}^{CC}(z) \sim -\frac{2}{\sqrt{z^2-1} (z + \sqrt{z^2-1})^n \left(1 - 1/(z + \sqrt{z^2-1})^{2n}\right)} \\ \times \left(\frac{\pi\sqrt{1-z^2}}{(z + \sqrt{z^2-1})^n} + \frac{2}{n^3} \left(\frac{(-1)^n}{z+1} - \frac{1}{z-1} \right) \right),$$

TABLE 4.1
 f_1 with $a = 0.5$, $k = 2$, $n = 30$, *Clenshaw–Curtis quadrature*.

b	Actual CC error	Asymptotic estimate
0.05	-0.102×10^1	-0.987×10^0
0.10	-0.163×10^{-1}	-0.163×10^{-1}
0.15	-0.389×10^{-3}	-0.389×10^{-3}
0.20	-0.114×10^{-4}	-0.114×10^{-4}

for $n \gg 1$. We might note that this is considerably more complicated algebraically than the corresponding expression for $k_n^{GL}(z)$ given in (3.1). We obtain a simplified version of (4.30) if we assume that n is even and also neglect the term $1/(z + \sqrt{z^2 - 1})^{2n}$. On observing that

$$(4.31) \quad \frac{\sqrt{1 - z^2}}{\sqrt{z^2 - 1}} = e^{\mp i\pi/2},$$

where the upper sign is taken for $\Im z > 0$ and the lower for $\Im z < 0$, we obtain

$$(4.32) \quad k_{n+1}^{CC}(z) \sim \frac{2}{(z + \sqrt{z^2 - 1})^n} \left(\frac{\pi e^{\pm i\pi/2}}{(z + \sqrt{z^2 - 1})^n} + \frac{4}{n^3(z^2 - 1)^{3/2}} \right),$$

assuming that n is large and even.

Consider the function $f_1(x) = x^2/((x - a)^2 + b^2)$. Its integral I_1 is given in (3.5). In Table 4.1 we give both the actual and the asymptotic estimate of the truncation error $E_{n+1}^{CC}f_1$ for $n = 30$, $a = 0.5$, and $b = 0.05(0.05)0.20$. The asymptotic estimate is obtained from, recalling (2.3),

$$(4.33) \quad E_{n+1}^{CC}f_1 = -\frac{1}{b}\Im(z_0^2 k_{n+1}^{CC}(z_0)),$$

with k_{n+1}^{CC} given by (4.32).

We observe that the asymptotic estimate agrees very well with the actual truncation error. Even when $b = 0.05$ the asymptotic estimate gives one significant digit. Furthermore, we observe that the absolute errors for 31-point Clenshaw–Curtis quadrature are not much different from those for 30-point Gauss–Legendre quadrature given in Table 3.1.

Let us now consider the integral I_2 as defined in (3.9). From (2.20) with $k = 1$ we have

$$(4.34) \quad E_{n+1}^{CC}f_2 = -\frac{1}{2} \sum_{l=0}^1 \binom{1}{l} \Re \left(\xi_0^{2-2l} \int_1^\infty s^{1-2l} (1 - 1/(\xi_0 s)^2) k_{n+1}^{CC}(z(s)) ds \right).$$

If we assume that n is even, then, since $b > 0$, we have from (3.7) and (4.32)

$$(4.35) \quad k_{n+1}^{CC}(z(s)) \sim \frac{2i\pi}{\xi_0^{2n} s^{2n}} + \frac{8}{n^3 \xi_0^n s^n (z^2(s) - 1)^{3/2}}.$$

But since from the definition of $z(s)$ in (2.8) we have

$$(4.36) \quad (z^2(s) - 1)^{1/2} = \frac{\xi_0 s}{2} \left(1 - \frac{1}{\xi_0^2 s^2} \right),$$

then

$$(4.37) \quad k_{n+1}^{CC}(z(s)) \sim \frac{2i\pi}{\xi_0^{2n} s^{2n}} + \frac{64}{n^3 \xi_0^{n+3} s^{n+3} (1 - 1/(\xi_0 s)^2)^3}.$$

TABLE 4.2
 f_2 with $a = -0.25$, $k = 1$, $n = 20$, Clenshaw–Curtis quadrature.

b	Actual CC error	Asymptotic estimate (4.40)
0.05	$+0.596 \times 10^{-2}$	$+0.606 \times 10^{-2}$
0.10	$+0.684 \times 10^{-3}$	$+0.689 \times 10^{-3}$
0.15	$+0.847 \times 10^{-4}$	$+0.851 \times 10^{-4}$
0.20	$+0.116 \times 10^{-4}$	$+0.116 \times 10^{-4}$

Substituting this into (4.34) gives

$$(4.38) \quad E_{n+1}^{CC} f_2 \sim - \sum_{l=0}^1 \binom{1}{l} \Re \left(\frac{\pi i}{\xi_0^{2n+2l-2}} \int_1^\infty \frac{(1 - 1/(\xi_0 s)^2)}{s^{2n+2l-1}} ds \right. \\ \left. + \frac{32}{n^3 \xi_0^{n+2l+1}} \int_1^\infty \frac{ds}{s^{n+2l+2} (1 - 1/(\xi_0 s)^2)^2} \right).$$

Since we are assuming that n is large, we see that the major contributions to these integrals come from the neighborhood of $s = 1$. If, in each integral, we replace the term $(1 - 1/(\xi_0 s)^2)$ by $(1 - 1/\xi_0^2)$, we find from (4.38) that

$$(4.39) \quad E_{n+1}^{CC} f_2 \sim - \sum_{l=0}^1 \binom{1}{l} \Re \left(\frac{\pi i (1 - 1/\xi_0^2)}{\xi_0^{2n+2l-2}} \int_1^\infty \frac{ds}{s^{2n+2l-1}} \right. \\ \left. + \frac{32}{n^3 \xi_0^{n+2l+1} (1 - 1/\xi_0^2)^2} \int_1^\infty \frac{ds}{s^{n+2l+2}} \right),$$

for $n \gg 1$. Evaluating these integrals gives the required asymptotic form for large n of the truncation error $E_{n+1}^{CC} f_2$. That is,

$$(4.40) \quad E_{n+1}^{CC} f_2 \sim - \sum_{l=0}^1 \binom{1}{l} \Re \left(\frac{\pi i (\xi_0^2 - 1)}{\xi_0^{2n+2l} (2n + 2l - 2)} \right. \\ \left. + \frac{32}{n^3 (\xi_0^2 - 1)^2 \xi_0^{n+2l-3} (n + 2l + 1)} \right).$$

In Table 4.2 we compare the actual truncation error in Clenshaw–Curtis quadrature with the asymptotic estimate as given by (4.40) in the particular case when $n = 20$, $a = -0.25$, and for $b = 0.05(0.05)0.20$.

Again we see that there is excellent agreement between the actual and asymptotic estimate of the truncation error, even for $n = 20$. From Table 4.2 we see that the absolute actual errors in 21-point Clenshaw–Curtis quadrature are about two or three times greater than the absolute actual errors for 20-point Gauss–Legendre quadrature as given in Table 3.2.

Finally let us consider the integral I_3 where f_3 is again defined with $k = 0$ and $\lambda = -1/2$ so that I_3 is given by (3.17). From (2.32) with $k = 0$ and $\lambda = -1/2$ we obtain

$$(4.41) \quad E_n f_3 = \frac{1}{\pi \sqrt{b}} \Re \left(e^{i\pi/4} \xi_0^{1/2} \int_1^\infty \frac{(1 - 1/(\xi_0 s)^2) k_n(z(s))}{(1 - 1/(\xi_0^2 s))^{1/2} (s - 1)^{1/2}} ds \right).$$

TABLE 4.3
 f_3 with $a = 0.75$, $\lambda = -0.5$, $k = 0$, $n = 30$, Clenshaw-Curtis quadrature.

b	Actual CC error	Asymptotic estimate(4.45)
0.05	-0.236×10^{-1}	-0.240×10^{-1}
0.10	-0.217×10^{-3}	-0.220×10^{-3}
0.15	-0.102×10^{-5}	-0.102×10^{-5}
0.20	$+0.610 \times 10^{-7}$	$+0.623 \times 10^{-7}$
0.25	$+0.439 \times 10^{-8}$	$+0.447 \times 10^{-8}$
0.30	$+0.185 \times 10^{-9}$	$+0.182 \times 10^{-9}$

Now we are considering $(n + 1)$ -point Clenshaw-Curtis quadrature with n even, so that from (4.37) we have

$$(4.42) \quad E_{n+1}^{CC} f_3 \sim \frac{2}{\pi\sqrt{b}} \Re \left(\frac{e^{3i\pi/4} \pi}{\xi_0^{2n-1/2}} \int_1^\infty \frac{(1 - 1/(\xi_0 s)^2) ds}{s^{2n} \sqrt{s-1} (1 - 1/(\xi_0^2 s))^{1/2}} \right. \\ \left. + \frac{32e^{i\pi/4}}{n^3 \xi_0^{n+5/2}} \int_1^\infty \frac{ds}{s^{n+3} \sqrt{s-1} (1 - 1/(\xi_0^2 s))^{1/2} (1 - 1/(\xi_0 s)^2)^2} \right).$$

Since we are assuming that $n \gg 1$ we again see that in each integral the main contribution comes from the neighborhood of $s = 1$ so that if we replace both $(1 - 1/(\xi_0^2 s))$ and $(1 - 1/(\xi_0 s)^2)$ by $(1 - 1/\xi_0^2)$ we find that

$$(4.43) \quad E_{n+1}^{CC} f_3 \sim \frac{2}{\pi\sqrt{b}} \Re \left(\frac{\pi e^{3i\pi/4} (\xi_0^2 - 1)^{1/2}}{\xi_0^{2n+1/2}} \int_1^\infty \frac{ds}{s^{2n} \sqrt{s-1}} \right. \\ \left. + \frac{32e^{i\pi/4}}{n^3 \xi_0^{n-5/2} (\xi_0^2 - 1)^{5/2}} \int_1^\infty \frac{ds}{s^{n+3} \sqrt{s-1}} \right).$$

Writing $s = 1/t$ gives

$$(4.44) \quad \int_1^\infty \frac{ds}{s^m \sqrt{s-1}} = \int_0^1 t^{m-3/2} (1-t)^{-1/2} dt = \frac{\sqrt{\pi} \Gamma(m-1/2)}{\Gamma(m)},$$

on recalling the definition of the Beta function; see Abramowitz and Stegun [1, section 6.2]. On using (4.44) in (4.43) and recalling Abramowitz and Stegun [1, section 6.1.47], we find, for n large and even, that

$$(4.45) \quad E_{n+1}^{CC} f_3 \sim \sqrt{\frac{2}{\pi b n}} \Re \left(\frac{\pi e^{3i\pi/4} (\xi_0^2 - 1)^{1/2}}{\xi_0^{2n+1/2}} + \frac{32\sqrt{2} e^{i\pi/4}}{n^3 \xi_0^{n-5/2} (\xi_0^2 - 1)^{5/2}} \right).$$

This is the required asymptotic truncation error estimate in this case.

In Table 4.3 we compare the actual truncation error in Clenshaw-Curtis quadrature with the asymptotic estimate (4.40) in the particular case when $n = 30$, $a = 0.75$, and for $b = 0.05(0.05)0.30$.

Again we see that the asymptotic estimates of the truncation error agree well with the actual truncation error.

5. Conclusion. From Tables 3.1 to 3.3 and 4.1 to 4.3 we see that, with only one exception, we have $|E_{n+1}^{CC} f / E_n^{GL} f| > 1$. (The exception being the function f_3 with

$$|k_{21}^{CC}(z)/k_{20}^{GL}(z)| = c$$

FIG. 5.1.

$n = 30$, $a = 0.75$, and $b = 0.15$.) From the analysis of the asymptotic estimates of the truncation errors, we see that the value of $E_n f$ depends mostly on the value of k_n in the neighborhoods of the points z_0 and $\bar{z}_0$. This suggests that it would be useful to determine contours in the z -plane where $|k_{n+1}^{CC}(z)/k_n^{GL}(z)| = c$ for various values of the constant c where we use the estimate (3.1) for $k_n^{GL}(z)$ and (4.32) for $k_{n+1}^{CC}(z)$. In Figure 5.1 we have plotted such contours for $n = 20$ and with c taking the values 2, 10, 100, and 1000. It is suggested that if z_0 and $\bar{z}_0$ lie well within the region bounded by the contour $c = 2$, then the absolute values of the truncation errors $E_{n+1}^{CC} f$ and $E_n^{GL} f$ will be comparable. We must note, however, how close the contours for $c = 10, 100$, and 1000 are to the contour with $c = 2$. This steep gradient implies that as $z_0, \bar{z}_0$ move away from the interval $[-1, 1]$, then Gauss–Legendre quadrature becomes much better than Clenshaw–Curtis quadrature. This is essentially the “kink” phenomenon as described by Weideman and Trefethen [10].

In Figure 5.2 we have plotted contours of $|k_{n+1}^{CC}(z)/k_n^{GL}(z)| = 10$ for n taking the values of 20, 30, and 40. We note that, as n increases, the size of the region around the interval $[-1, 1]$, where Clenshaw–Curtis and Gauss–Legendre quadrature may give comparable truncation errors, diminishes. This is consistent with the findings of Weideman and Trefethen [10].

Since we are dealing with integrals arising from the boundary integral method, let us recall that many methods have been used for their numerical evaluation which make use of a transformation of the variable of integration in order to cope with a singularity close to the interval of integration. A recent paper by Johnston, Johnston, and Elliott [6] makes a comparison of these transformations and concludes that the so-called “sinh-transformation,” introduced by Johnston and Elliott [7], invariably

$$|k_{n+1}^{CC}(z)/k_n^{GL}(z)| = 10$$

FIG. 5.2.

outperforms the others. Elliott and Johnston [5, theorem 3.4] have shown that the effect of the sinh-transformation is to replace the original singularities by ones that are “further away” from the interval $(-1, 1)$. That is, the transformed integrand will have singularities in regions where Gauss–Legendre quadrature is likely to outperform Clenshaw–Curtis quadrature.

So let us conclude by considering the effects of the sinh-transformation for both Clenshaw–Curtis and Gauss–Legendre quadratures. We shall compare the asymptotic error estimates for just one example; the function f_1 with $k = 2$; see (1.2). From (3.3), the error for n -point Gauss–Legendre quadrature is given by

$$(5.1) \quad E_n^{GL} f_1 \sim -\frac{c_n}{b} \Im \left\{ \frac{z_0^2}{(z_0 + \sqrt{z_0^2 - 1})^{2n+1}} \right\},$$

for $n \gg 1$. From (4.32) and (4.33) we have, for $(n + 1)$ -point Clenshaw–Curtis quadrature with n even, that

$$(5.2) \quad E_{n+1}^{CC} f_1 \sim -\frac{1}{b} \Im \left\{ z_0^2 \left(\frac{2\pi i}{(z_0 + \sqrt{z_0^2 - 1})^{2n}} + \frac{8}{n^3(z_0^2 - 1)^{3/2}(z_0 + \sqrt{z_0^2 - 1})^n} \right) \right\}.$$

The sinh-transformation is given by

$$(5.3) \quad x = a + b \sinh(\mu u - \eta),$$

where, on choosing

$$(5.4) \quad \mu = (\operatorname{arcsinh}((1+a)/b) + \operatorname{arcsinh}((1-a)/b))/2,$$

and

$$(5.5) \quad \eta = (\operatorname{arcsinh}((1+a)/b) - \operatorname{arcsinh}((1-a)/b))/2,$$

the original interval of integration $(-1, 1)$ is mapped onto $(-1, 1)$ again, so that the *same* quadrature rule can be used on the transformed integral as on the original integral. In [7], it has been shown that for Gauss–Legendre quadrature the reduction in the truncation error can be dramatic. Consider

$$(5.6) \quad I_1 = \int_{-1}^1 \frac{x^2 dx}{(x-a)^2 + b^2}.$$

Under the transformation given by (5.3) to (5.5) we have

$$(5.7) \quad I_1 = \frac{\mu}{b} \int_{-1}^1 \frac{x^2(u) du}{\cosh(\mu u - \eta)}.$$

The transformed integral has simple poles at points $w_k, \bar{w}_k$, for all $k \in \mathbf{N}_0$, where

$$(5.8) \quad w_k := \frac{\eta}{\mu} + i \frac{(k+1/2)\pi}{\mu}.$$

The main contribution to the truncation error will come from the pair of simple poles at $w_0, \bar{w}_0$, so let us approximate to the integral I_1 of (5.7) by I_1^{tr} , say, where

$$(5.9) \quad I_1^{tr} := \int_{-1}^1 f_1^{tr}(u) du := \frac{\pi}{b\mu} \int_{-1}^1 \frac{x^2(u) du}{(u-w_0)(u-\bar{w}_0)}.$$

The residue of the function f_1^{tr} at w_0 is given by $x^2(w_0)/(ib)$, and it is easy to show from (5.3) and (1.6) that

$$(5.10) \quad x(w_0) = a + ib = z_0.$$

For n -point Gauss–Legendre quadrature applied to I_1^{tr} , the truncation error is given by

$$(5.11) \quad E_n^{GL} f_1^{tr} \sim -\frac{2c_n}{b} \Im \left\{ \frac{z_0^2}{(w_0 + \sqrt{w_0^2 - 1})^{2n+1}} \right\}.$$

Again, for n large and even, the truncation error for $(n+1)$ -point Clenshaw–Curtis quadrature applied to I_1^{tr} is

$$(5.12) \quad E_{n+1}^{CC} f_1^{tr} \sim -\frac{2}{b} \Im \left\{ z_0^2 \left(\frac{2\pi i}{(w_0 + \sqrt{w_0^2 - 1})^{2n}} + \frac{8}{n^3(w_0^2 - 1)^{3/2} (w_0 + \sqrt{w_0^2 - 1})^n} \right) \right\}.$$

TABLE 5.1
 f_1 with $a = 0.925$ and $k = 2$.

b	Untransformed integral		Transformed integral	
	21-point CC (5.2)	20-point GL (5.1)	20-point GL (5.11)	21-point CC (5.12)
0.05	+0.605	-0.496	-0.342×10^{-9}	$+0.708 \times 10^{-8}$
0.15	-0.113×10^{-3}	$+0.821 \times 10^{-4}$	-0.891×10^{-14}	-0.131×10^{-9}
0.25	$+0.171 \times 10^{-5}$	-0.219×10^{-6}	-0.246×10^{-16}	-0.310×10^{-11}
0.35	$+0.373 \times 10^{-7}$	$+0.130 \times 10^{-8}$	-0.316×10^{-18}	-0.210×10^{-12}
0.45	-0.297×10^{-8}	$+0.860 \times 10^{-11}$	-0.387×10^{-20}	-0.208×10^{-13}

TABLE 5.2
 f_1 with $a = 0.925$, $k = 2$, and $n = 20$.

b	$ E_{21}^{CC} f_1 / E_{20}^{GL} f_1 $
0.05	1.22
0.15	1.38
0.25	7.83
0.35	28.6
0.45	345

In Table 5.1 we give these truncation error estimates for the particular case when $n = 20$, $a = 0.925$, and $b = 0.05(0.10)0.45$.

From the second and third columns of Table 5.1, we see that the modulus of the errors in Clenshaw-Curtis and Gauss-Legendre quadratures are comparable for $b \leq 0.15$ with Gauss-Legendre quadrature giving smaller truncation errors than Clenshaw-Curtis quadrature as b increases. In order to highlight the improvement that the transformation can give, we have shown, in the next column, the truncation errors for Gauss-Legendre quadrature after the application of the sinh-transformation. With a reduction of the truncation error of the order of 10^{-10} , this may be considered to be dramatic. In the last column of Table 5.1 we have given the truncation errors in the transformed integral with Clenshaw-Curtis quadrature. Comparing these errors with those of the untransformed integral, as given in the second column, we see that the improvement here is roughly of the order of 10^{-6} .

In Table 5.2, we tabulate the ratio of the modulus of the truncation errors in 21-point Clenshaw-Curtis quadrature with those for 20-point Gauss-Legendre quadrature, in the untransformed case.

We see that the ratio increases with b , which is in keeping with the predictions of Figure 5.1. If we imagine a vertical line drawn through $a = 0.925$, we see that the line lies within the curve $c = 2$ for small values of b but, as b increases, c increases dramatically, and this is reflected by the ratios given in Table 5.2.

Although one example *proves* nothing, let us repeat that the effect of the sinh-transformation is to put the singularities of the integrand further away from the interval of integration $(-1, 1)$. It should be remembered that the boundary element method also requires the evaluation of integrals whose integrands have singularities well removed from $(-1, 1)$. In this case Gauss-Legendre quadrature is much superior to Clenshaw-Curtis quadrature. Since it is convenient, if possible, to have one quadrature rule for *all* situations, then, in the context of boundary integral methods, we propose to continue with Gauss-Legendre quadrature together with the sinh-transformation for nearly singular integrals.

But Trefethen [9] and Weideman and Trefethen [10] are absolutely correct; when the integrand has its singularities “close enough” to the interval of integration, then

Clenshaw–Curtis quadrature and Gauss–Legendre quadrature do indeed give comparable truncation errors.

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REFERENCES

- [1] M. ABRAMOWITZ AND I. A. STEGUN, *Handbook of Mathematical Functions*, Dover Publications, New York, 1970.
- [2] C. A. BREBBIA AND J. DOMINGUEZ, *Boundary Elements, An Introductory Course*, 2nd ed., Computational Mechanics Publications, Southampton, 1992.
- [3] J. D. DONALDSON AND D. ELLIOTT, *A unified approach to quadrature rules with asymptotic estimates of their remainders*, SIAM J. Numer. Anal., 9 (1972), pp. 573–602.
- [4] D. ELLIOTT, *The evaluation and estimation of the coefficients in the Chebyshev series expansion of a function*, Math. Comput., 18 (1964), pp. 274–284.
- [5] D. ELLIOTT AND P. R. JOHNSTON, *Error analysis for a sinh transformation used in evaluating nearly singular boundary element integrals*, J. Comput. Appl. Math., 203 (2007), pp. 103–124.
- [6] B. M. JOHNSTON, P. R. JOHNSTON, AND D. ELLIOTT, *A sinh transformation for evaluating two-dimensional nearly singular boundary element integrals*, Internat. J. Numer. Methods Engrg., 69 (2007), pp. 1460–1479.
- [7] P. R. JOHNSTON AND D. ELLIOTT, *A sinh transformation for evaluating nearly singular boundary element integrals*, Internat. J. Numer. Methods Engrg., 62 (2005), pp. 564–578.
- [8] J. C. MASON AND D. C. HANDSCOMB, *Chebyshev Polynomials*, CRC, Boca Raton, FL, 2003.
- [9] L. N. TREFETHEN, *Is Gauss quadrature better than Clenshaw-Curtis?*, SIAM Rev., 50 (2008), pp. 67–87.
- [10] J. A. C. WEIDEMAN AND L. N. TREFETHEN, *The kink phenomenon in Fejér and Clenshaw-Curtis quadrature*, Numer. Math., 107 (2007), pp. 707–727.