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ERROR ESTIMATES FOR SOME QUADRATURE FORMULAE

by

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Error Estimates

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Introduction

In the technical report TR/25 we developed continued fractions for a number of the so-called special functions of mathematics. We also derived rigorous error estimates for the rational function approximations we obtained by truncating these continued fractions. Now it is known that quadrature formulae are centred on the partial fraction expansions of truncated continued fractions, so in this paper we will extend our analysis and estimate the errors in using certain quadrature formulae. We first derive the quadrature formulae related to the Laplace transforms of Bessel functions and then develop the error analysis for them. We will demonstrate that the error estimates can be very effective, and that for the special cases we consider are relatively simple to calculate.

This paper is a sequel to the technical report TR/25, and relations in that report are referenced directly. The general form of our continued fractions in TR/25 was

$$Y = \frac{c_1}{d_1}+\frac{c_2}{d_2}+ - - - + \cfrac{c_n}{d_n - \cfrac{Y_n}{Y_{n-1}}}$$

where c_i, d_i denote polynomials in s. Writing the n convergent of Y(s) as the rational function $\frac{C_n(s)}{D_n(s)}$, we found the error

$$Y - \frac{C_n}{D_n} = \frac{Y_n}{D_n},$$

We also showed that for the special functions, Laquerre, Hermite, Legendre and the Laplace transform of a Bessel function, this error term can often be replaced by an expression of the form

$$w(s)e^{2i\phi}[1-\tanh(\theta+ i\phi)] - 2w(s)e^{-2\theta(s)}$$

where w(s) is the weight function.

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Clearly whenever Y(s) is replaced by $\frac{C_n(s)}{D_n(s)}$ we can attempt to estimate the error incurred. In particular awkward terms in integrals can frequently be dealt with by replacing them by $\frac{C_n(s)}{D_n(s)}$ and it is with this application that we will be primarily concerned. With the results in TR/25 as our basis, we could establish most of the common Gaussian quadrature formulae with error estimates. But as we indicated above we will concentrate on just a few. Let us start by deriving the Gauss-Legendre quadrature formula for the definite integral

$$\int_{-1}^{1} f(x)dx.$$

21. Quadrature Formulae

Given a function f(x) regular in a domain D containing the interval [-1,1]. We write this function f(x) as a Cauchy integral

$$f(x) = \frac{1}{2\Pi i}\int_c \frac{f(s)}{s-x}ds \quad , \tag{21.1}$$

where the path of integration C encloses the point x, C is chosen to lie in D.

Integrating from -1 to 1 gives

$$\int_{-1}^{1} f(x)\,dx = \frac{1}{2\Pi i}\int_c f(s)\log\left(\frac{s+1}{s-1}\right) ds \ . \tag{21.2}$$

But log $\left(\frac{s+1}{s-1}\right)$ can be expressed as the *C.F.(4.6)* and from (4.10)

$$\frac{1}{2}\log\left(\frac{s+1}{s-1}\right) = \frac{C_n(s)}{n!P_n(s)} + \frac{Q_n(s)}{P_n(s)} = \sum_{r=1}^{n} \frac{A_r}{s-x_r} + \frac{Q_n(s)}{P_n(s)} \tag{21.3}$$

where the x denote the roots of the Legendre polynomials,

$$A_r^{-1} = (1-x_r^2)[P_n'(x_r)]_2$$

and $P_n(s)$, $Q_n(s)$ are the Legendre functions of the first and second kinds.

Hence

$$\int_{-1}^{1} -f(x)\,dx = \frac{2}{2\Pi}\sum_{r=1}^{n} \int_C f(s)\frac{A_r}{s-x_r}ds + \frac{2}{2\Pi}\int_C f(s)\frac{Q_n(s)}{P_n(s)}ds$$
$$= 2\sum_{r=1}^{n} A_r f(x_r) + E_n$$

(21.4)

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the usual Gauss-Legendre quadrature formula, but with a precise expression for the error E_n .

The above immediately generalises to include quadrature formulae for integrals containing a weight function w(x), as has been pointed out by Takahasi and Mori [∯7]. Given a function f(x) regular in a domain D containing the interval [a,b] which may be infinite, and with w(x) regular in (a,b), we write

$$\int_a^b f(x)w(x)\,dx = \frac{1}{2\Pi i}\int_C f(s)\int_a^b \frac{w(x)}{s-x}\,dx\,ds. \tag{21.5}$$

Setting

$$\int_a^b \frac{w(x)}{s-x}\,dx = \sum_{r=1}^{n} \frac{w_{rn}}{s-x_{rn}} + \frac{Y_n(s)}{D_n(s)} \tag{21.6}$$

which we obtain from the n^{th} convergent of the J fraction for the function on the right, the x_r being the roots of the denominator polynomials $D_n(s)$, we find

$$\int_a^b f(x)w(x)\,dx = \sum_{r=1}^{n} w_{rn} f(x_{rn}) + E_n, \tag{21.7}$$

where again we have a precise expression for the error

$$E_n = \frac{1}{2\Pi i}\int_c f(s)\frac{Y_n(s)}{D_n(s)}\,ds. \tag{21.8}$$

The expansion (21.6) of the integral

$$Y(s) \equiv \int_a^b \frac{w(x)}{s-x}\,dx$$

is obtained from the J fraction for Y(s). This continued fraction can be constructed either directly, by forming successively the linear relations equivalent to the fraction, or, when Y(s) satisfies a first order linear differential equation, by the method developed in §11 of TR/26. The J fractions required for the common quadrature formulae are known.

A variety of techniques have been used to estimate the error E_n of the common quadrature formulae, for example Davis and Rabinowitz [18] give error bounds in terms of the product of norms of the integral operator and the integrand, while Takahasi and Mori [4.2] estimate $|E_n|$ numerically by an approximate steepest descent method which they claim is fairly accurate. Our approach will be direct. In TR/25 we developed estimates for the truncation errors of a number of continued fractions, some were both simple and reliable, we will place these in (21.8) to estimate the E_n of certain quadrature formulae.

22. Error Estimates for Two Special Cases.

In this section we obtain estimates depending explicitly on n for the error E_n for the Gauss-Legendre and Gauss-Chebyshev formulae, these being special cases of the more general quadrature formula related to Bessel functions considered in the next section.

a) Gauss -Legendre quadrature.

Consider the Gauss-Legendre formula (21.4) that we have just derived

$$\int_{-1}^{1} f(x)\,dx = 2\sum_{r=1}^{n} A_r f(x_r) + E_n, \tag{22.1}$$

where

$$E_n = \frac{2}{2\Pi i}\int_C f(s)\frac{Q_n(s)}{P_n(s)}ds. \tag{22.2}$$

A useful approximation for the ratio of the Legendre functions is from (4.14) in TR/25, s= cosh ζ,

$$\frac{Q_n(s)}{P_n(s)} \sim \Pi e^{-(2n+1)\zeta} = \frac{\Pi}{[s+\sqrt{s^2-1}]^{2n+1}}. \tag{22.3}$$

Hence

$$E_n = \frac{1}{i}\int_C f(s)e^{-(2n+1)\zeta}ds \tag{22.4}$$

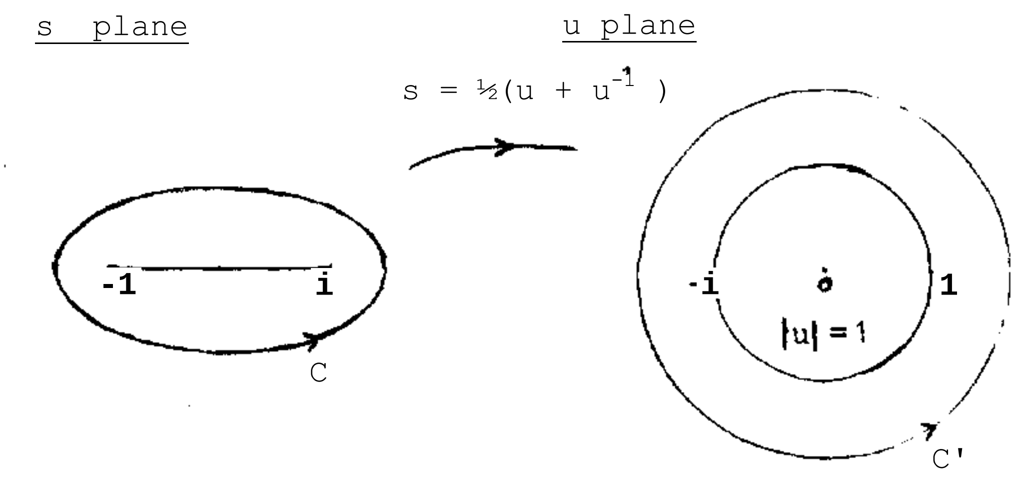
or

$$= \frac{1}{i}\int_c f(s)\frac{ds}{[s+\sqrt{s^2-1}]^{2n+1}}. \tag{22.5}$$

This latter integral can be rearranged to advantage by replacing s by $\frac{1}{2}(u+u^{-1})$, for then $u = s+\sqrt{s^2-1}$ and

$$E_n = \frac{1}{2i}\int_{C'} f\left(\frac{1}{2}(u+u^{-1})\right).\left(\frac{1}{u^{2n+1}} - \frac{1}{u^{2n+3}}\right)du \tag{22.6}$$

where C is mapped in the u plane on to C'.



This mapping of the s plane on to the u plane is particularly-convenient for it completely removes the branch cut, and gives a contour C' which we can expand or contract. The contribution to (22.6) from the origin (or infinity) can he deduced if the Laurent series

$$f\left(\frac{1}{2}(u + u^{-1})\right) = \sum_{k=-\infty}^{\infty} a_k u^k \tag{22.7}$$

can he evaluated.

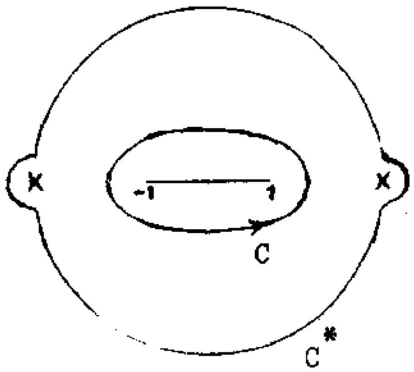
Thus to estimate E_n we have the choice of evaluating one of the simple contour integrals (22.4) and (22.6). Let us take two elementary examples to illustrate results that we have obtained from these integrals. Our estimates of E are impressive and we suspect are typical.

1) $\int_1^1 \sec \frac{\Pi}{4} x dx$, With $f(s) = \sec \frac{\Pi}{4} s$, (22.4) becomes

$$E_n = \frac{1}{i} \int_C \frac{e^{-(2n+1)\zeta}}{\cos \frac{\Pi}{4} s} ds.$$

We see that the integrand has simple poles at $s = \pm 2(2m+1)$, where m is a positive integer. For a first approximation to

8.



this integral let us expand C beyond the first poles, so that

$$En \simeq 2\Pi i \begin{bmatrix} \text{residues from} \\ \text{poles at } \pm 2 \end{bmatrix} + \frac{1}{i}\int_{C^*}$$

and discard the contribution from C . We find

$$\underline{En \simeq 16 e^{-(2n+1)1.317}} \qquad (22.8)$$

$$\int_{-1}^{1} \sec \frac{\Pi}{4} x dx = \frac{4}{\Pi} \log \left(\frac{\sqrt{2}+1}{\sqrt{2}-1} \right) = 2.24439940 \quad 9$$

n	G - L quad(22.1)	E_n	Estimate (22.8)
2	2.22483966	1.96(-2)	2.21(-2)
3	2.24294052	1.46(-3)	1.59(-3)
4	2.24429263	1.07(-4)	1 .14(-4)
5	2.24439165	7.76(-6)	8.18(-6)
6	2.24439885	5.62(-7)	5.88(-7)
7	2.24439937	4.06(-8)	4.22(-8)
8	2.24439941	2.93(-9)	3.03(-9)

From these tabulated values we see that (22.8) provides a good estimate of E_n even for n small,

2) $\underline{\int_{-1}^{-} e^{tx} dx.}$ To illustrate (22.6) this example almost suggests itself, for (22.6) becomes

$$E_n \simeq \frac{1}{2i}\int_{C'} e^{\frac{t}{2}(u+u^{-1})} \cdot \left(\frac{1}{u^{2n+1}} - \frac{1}{u^{2n+3}} \right) du$$

and as $e^{\frac{t}{2}(u+u^{-1})} = \sum_{-\infty}^{\infty} T_k(t) u^k$, we immediatel y deduce

$$E_n \simeq \Pi(I_{2n}(t) - I_{2n+2}(t)]. \qquad (22.9)$$

$$\int_{-1}^{1} e^{3x}\, dx = \frac{1}{3}\left(e^{3} - e^{-3}\right) = 6.678583285$$

n	G - L quad (22.1)	E_n	Estimate (22.9)
2	5.82915488	8.49(-1)	9.55(-1)
3	6.61789733	6.07(-2)	6.56(-2)
4	6.67622947	2.35(-3)	2.50(-3)
5	6.67852591	5.74(-5)	6.01(-5)
6	6.67858233	0.96(-6)	1.00(-6)
7	6.67858327	1.17(-8)	1.21(-8)
8	6.67858328	1.13(-10)	1.12(-10)

Again for n small in (22.9) we have a good estimate of E_n.

By making use of the asymptotic formula

$$I_n(t) \sim \frac{1}{\sqrt{2\Pi}} \frac{e^{\sqrt{n^2+t^2} - n \sinh^{-1}\frac{n}{t}}}{(n^2+t^2)^{\frac{1}{4}}} \left\{ 1 + \frac{3t^2 - 2n^2}{24(n^2+t^2)^{3/2}} = + \ldots \right\}$$

see for example Abramowitz and Segun [9.7.7], we can obtain an expression for the error E in terms of more elementary functions

$$E_n(t) \approx \sqrt{\frac{\Pi}{2}}\, \frac{e^{\sqrt{4n^2++t^2} - 2n \sinh^{-1}\frac{2n}{t}}}{(4n^2+t^2)^{\frac{1}{4}}}.$$

This expression gives, for t = 3, values which are not very different to those we obtained using (22.9).

The first of these examples illustrates the important point that usually it will be the singularities of f(s) nearest to the cut (-1,1) that will dominate E as n is increased. When f(s) has only poles outside C, we can replace (22.5) by

$E_n \sim -2\pi i$ [residues from poles nearest to cut].

In particular a pole at s contributes to this expression for E_n

$$-\frac{2\Pi}{h'(s_o)\left(s_o + \sqrt{s_o^2 - 1}\right)^{2n+1}},$$

where we have written $\frac{1}{h(s)}$ in place of f(s) .

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b) Gauss-Chebyshev quadrature.

From (21.5) we $\mathcal{L}$see that

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx = \frac{1}{2\Pi\Pi} \int_c f(s) \int_{-1}^{1} \frac{1}{s-x} \frac{dx}{\sqrt{1-x^2}} ds. \qquad (22.10)$$

But

$$\int_{-1}^{1} \frac{1}{s-x} \frac{dx}{\sqrt{1-x^2}} = \int_{o}^{\Pi} \frac{d\phi}{s-\cos\phi} = \Pi \mathcal{L}\ I_o(t) = \frac{\Pi}{\sqrt{s^2-1}} \qquad (22.11)$$

Now Murphy [4.1] has examined the error in approximating $\frac{1}{\sqrt{s^2-1}}$ by the nth convergent of the C.F. which matches its series for s large.

$$\frac{1}{\sqrt{s^2-1}} - \frac{1}{s-} \frac{1}{2s-} - \frac{1}{2s-} \frac{1}{2s} ----. \qquad (22.12)$$

He found that with s = cosh ζ and $\zeta = i\theta$

$$\frac{1}{\sqrt{s^2-1}} - \frac{C_n(s)}{D_n(s)} = \frac{e^{-n\zeta}}{\sinh\ \zeta inh\zeta c} - \frac{2e^{-2n\zeta}}{\sqrt{s^2-1}} \qquad (22.13)$$

where D_n (s) = cos $n\theta$ and C_n $\frac{\sin n\theta}{\sin\theta}$ and are the Chebyshev polynomials of the first and second kinds. Further he expanded the ratio $\frac{C_n}{D_n}$ in partial fractions,

$$\frac{C_n(s)}{D_n(s)} = \frac{1}{n} \sum_{r=1}^{n} \frac{1}{s - \cos\frac{(r-\frac{1}{2})\Pi}{n}}. \qquad (22.14)$$

Substituting (22.13) in

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx = \frac{\Pi}{2\Pi i} \int_C f(s) \frac{1}{\sqrt{s^2-1}} ds \qquad (22.15)$$

gives the quadrature, with $\phi r \equiv \frac{(r-\frac{1}{2})\Pi}{n}$

$$\int_0^{\Pi} f(\cos\phi)\,d\phi = \frac{\Pi}{n}\sum_{r=1}^{n} f(\cos\phi_r) + E_n \;, \qquad (22.16)$$

where

$$E_n \simeq \frac{1}{i}\int_C f(s)\,\frac{e^{-2n\zeta}}{\sqrt{s^2-1}}\,ds. \qquad (22.17)$$

The substitution, $s=\frac{1}{2}(u+u^{-1})$, that we used to obtain (22.6) also considerably simplifies this contour integral. Denoting, as before, the contour that C maps onto in the u plane by C', we deduce

$$En \simeq \frac{1}{i}\int_{C'} f(\frac{1}{2}(u + u-1))\,\frac{1}{u2n+1}\,du. \qquad (22.18)$$

Again we have found a simple and convenient starting point for analysing the error E_n.

These two quadrature formulae Gauss-Legendre and Gauss-Chebyshev are of course closely related both being special cases of the following.

 12.

23. The Quadrature Formula for $\int_{-1}^{1} f(x)(1-x^2)^{v-\frac{1}{2}}\,dx$.

We now construct a quadrature formula with the weight function

$$w(x) = (1-x^2)^{v-\frac{1}{2}} \quad . \tag{23.1}$$

Since, see (5.20) with n = 0, for $Rv>-\frac{1}{2}$

$$\int_{-1}^{1} \frac{(1-x^2)^{v-\frac{1}{2}}}{s-x}\,dx = 2^v\sqrt{\Pi}\Gamma(v+\frac{1}{2}) \quad \mathcal{L}\,\frac{I_v(t)}{t^v} \quad , \tag{23.2}$$

the essential step is to use the C.F.(5.6) and replace

$2^v\Gamma(v+1)\,\mathcal{L}\,\frac{I_v}{t^v}$ by the n^{th} convergent of (5.6) together with an error term,

$$\int_{-1}^{1} \frac{(1-x2)v-\frac{1}{2}}{s-x}dx = \frac{\sqrt{\Pi}\Gamma(v+\frac{1}{2})}{\Gamma(v+1)}\left[\frac{Cn(s)}{Dn(s)}+\frac{Y}{}\right] \tag{23.3}$$

By (5.21) the n conΓvergent in partial fractions is

$$\frac{C_n(s)}{D_n(s)} = \frac{\Gamma\big(2v+n\big)}{\Gamma(2v)}\frac{2v}{n!}\sum_{r=1}^{n}\frac{A_{rn}}{s-x_{rn}} \tag{23.4}$$

where $A_{rn}^{-1} = (1-x_{rn}^2)[G_n^v(x_{rn})]2$ and the x_{rn} are the rots of the Gegendauer polynomials $G_n^v(x)$. for the error term we use (5.29)

$$\frac{Y_n(s)}{D_n(s)} = \frac{2\sqrt{\Pi}\,\Gamma(v+1)}{\Gamma(v+\frac{1}{2})}\frac{(s^2-1)^{v-\frac{1}{2}}}{[s+\sqrt{s^2-1}]^{2(n+v)}}. \tag{23.5}$$

Making use of the doubling formula $\Gamma(v)\Gamma(v+\frac{1}{2}) = \sqrt{\Pi}2^{-2v+1}\Gamma(2v)$, we deduce

$$\int_{-1}^{1} \frac{(1-x^2)^{v-\frac{1}{2}}}{s-x}\,dx = \sum_{r=1}^{n}\frac{w_{rn}}{s-x_{rn}} + \frac{\sqrt{\Pi}\Gamma(v+\frac{1}{2})}{\Gamma(v+1)}\frac{Y_n(s)}{D_n(s)} \tag{23.6}$$

Where $w_{rn} = \frac{\Pi\, 2^{2-2v}\,\Gamma(2v+n)}{\Gamma(v)^2 .n!} A_{rn}$.

This is the required expansion (21.6) and hence by (21.7)

$$\int_{-1}^{1} f(x)(1-x^2)^{v-\frac{1}{2}}\,dx = \sum_{r=1}^{n} w_{rn}\, f(x_{rn}) + E_n, \tag{23.7}$$

where the error term

$$E_n = \frac{1}{i}\int_C f(s)\,\frac{(s^2-1)\,v-\frac{1}{2}}{[s+\sqrt{s^2-1}]^{2(n+v)}}\,ds \tag{23.8}$$

$$= \frac{1}{i}\int_{C'} f(\tfrac{1}{2}(u+u^{-1}))\,\frac{(u-u-1)\,2v}{2^{2v}\,u^{2(n+v)+1}}\,du. \tag{23.9}$$

Again we have made the substitution $s=\frac{1}{2}(u+u)^{-1}$, C and C' are the same contours as we used in the previous section. The n is still in a suitable position for deriving asymptotic estimates for the error.

If we take $f(x) = e^{tx}$ in (23.7), we get that

$$2^v\sqrt{\Pi}\,\Gamma(v+\tfrac{1}{2})\,\frac{I_v(t)}{t^v} = \sum_{r=1}^{n} w_{rn}\, e^{x_{rn}t} + E_n \tag{23.10}$$

which is in essence our result (5.22). Quadrature results can be regarded as an extension of previous results obtained by inverting Laplace transforms.

14.

Conclusion

In this short report we have deduced some useful simple complex integrals that approximately give the errors E_n of the Gauss-Legendre and Gauss-Chebyshev quadrature formulae. We also showed that these were special cases of a more general result. The potential of these complex integrals was illustrated by deriving some specific error estimates as functions of n.

It is often desirable to be able to choose the number of terms n in a quadrature formula in advance, in particular when approximating to an integral containing parameters or to a function that is one in a sequence of calculations. Our numerical results indicate that the value of n required to achieve a given accuracy could be accurately selected using our estimates.

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