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# Estimates of the Error in Gauss-Legendre Quadrature for Double Integrals

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**Abstract**

Error estimates are a very important aspect of numerical integration. It is desirable to know what level of truncation error might be expected for a given number of integration points. Here, we determine estimates for the truncation error when Gauss-Legendre quadrature is applied to the numerical evaluation of two dimensional integrals which arise in the boundary element method. Two examples are considered; one where the integrand contains poles, when its definition is extended into the complex plane, and another which contains branch points. In both cases we obtain error estimates which agree with the actual error to at least one significant digit.
*Keywords:* Double integrals, Gauss-Legendre quadrature, Numerical Integration

## 1. Introduction

In a recent paper [1], the authors have considered, in the context of the boundary integral method [2], the evaluation of double integrals of the form

$$\int_{-1}^{1}\int_{-1}^{1}\frac{\phi(x,u)\,dx\,du}{((x-x_0)^2+(u-u_0)^2+b^2)^{\alpha}}, \tag{1.1}$$

where $-1 \le x_0, u_0 \le 1$, $0 < b < 1$, $\phi$ is a bi-quadratic function and $\alpha \in \mathbb{R}^+$. In order to evaluate this integral approximately, the authors have used Gauss-Legendre quadrature in each of the variables of integration.

Integrals of the form of equation (1.1) arise in many applications of the boundary element method, especially when the potential or flux is required near a boundary. This occurs in the

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study of thin structures [3], sensitivity problems [4], contact problems [5] and displacement around open crack tips [6].

In the past the authors have determined expressions for the truncation error when evaluating integrals which are the single variable analogue of equation (1.1). The truncation errors of these types of integrals were studied for numerical evaluation with Gauss-Legendre quadrature [7] as well as with a sinh transformation [8, 7] for small values of the parameter $b$. Further, error estimates for integrals involving the Hankel function, evaluated with Gauss-Legendre quadrature, have also been obtained [9].

The purpose of this paper is firstly, to give an expression for the truncation error in the evaluation of the integral (1.1) and secondly, to see how this can be used to give asymptotic estimates for these errors. We shall consider, in detail, two particular examples in which we shall compare the actual truncation errors with the asymptotic estimates.

## 2. The quadrature rule and its remainder

Consider first the integral $I$ given by

$$I := \int_{-1}^{1} \Big( \int_{-1}^{1} f(x,u)\, dx \Big)\, du = \int_{-1}^{1} \Big( \int_{-1}^{1} f(x,u)\, du \Big)\, dx, \tag{2.1}$$

for some appropriate function $f$. Let us recall, from Donaldson and Elliott [10], the expression for $n$-point Gauss-Legendre quadrature, where $n \in \mathbb{N}$. We have

$$\int_{-1}^{1} f(x)\, dx = \sum_{k=1}^{n} \lambda_{k,n} f(x_{k,n}) + \frac{1}{2\pi i} \int_{C_z} k_n(z) f(z)\, dz. \tag{2.2}$$

Here $x_{k,n}$, $k = 1(1)n$, are the zeros of the Legendre polynomials $P_n$ and $\lambda_{k,n}$, $k = 1(1)n$, are the corresponding weights or Christoffel numbers. On the assumption that the definition of $f$ may be continued into the complex $z$ - plane, where $z = x + iy$, we have expressed the remainder, or truncation error, of the quadrature rule as a contour integral. The contour $C_z$ encloses the interval $-1 \leq \Re z \leq 1$ and is such that the function $f$ is analytic on and within $C_z$. The function $k_n$ is independent of $f$ and depends only on the fact that we are using $n$-point Gauss-Legendre quadrature. For $z \notin [-1, 1]$ it is defined by

$$k_n(z) := \Pi_n(z)/P_n(z) \tag{2.3}$$

where

$$\Pi_n(z) := \int_{-1}^{1} \frac{P_n(t)\, dt}{z - t}. \tag{2.4}$$

We have that $k_n$ is analytic in the complex $z$-plane with the interval $-1 \le \Re z \le 1$ deleted.

We shall now derive an $M \times N$ point Gauss-Legendre quadrature rule for the double integral $I$, defined in (2.1). For a given $x \in [-1,1]$ let us first consider the integral $\int_{-1}^{1} f(x,u)\,du$. From (2.2) and (2.3) we have

$$\int_{-1}^{1} f(x,u)\,du = \sum_{k=1}^{N} \lambda_{k,N} f(x, u_{k,N}) + R_{N,1}(x) \tag{2.5}$$

where, if we write $w = u + iv$, the remainder $R_{N,1}(x)$ is given by

$$R_{N,1}(x) := \frac{1}{2\pi i}\int_{C_w} k_N(w) f(x,w)\,dw. \tag{2.6}$$

The contour $C_w$ encloses the interval $-1 \le u = \Re w \le 1$ and is such that $f(x,w)$ is analytic on and within $C_w$. From (2.1) and (2.5) we have

$$\begin{aligned} I &= \int_{-1}^{1}\Big(\int_{-1}^{1} f(x,u)\,du\Big)\,dx \qquad (2.7)\\ &= \sum_{k=1}^{N}\lambda_{k,N}\int_{-1}^{1} f(x,u_{k,N})\,dx + \int_{-1}^{1} R_{N,1}(x)\,dx. \end{aligned}$$

We shall now apply an $M$-point Gauss-Legendre quadrature rule to the integral $\int_{-1}^{1} f(x, u_{k,N})\,dx$. On defining

$$R_{M,2}(u) := \frac{1}{2\pi i}\int_{C_z} k_M(z) f(z,u)\,dz, \tag{2.8}$$

where the contour $C_z$ encloses the interval $-1 \le x = \Re z \le 1$ and is such that, for all $u \in [-1,1]$, the function $f(z,u)$ is analytic on and within $C_z$ we find, from (2.7), that

$$I = \sum_{k=1}^{N}\lambda_{k,N}\Big(\sum_{j=1}^{M}\lambda_{j,M} f(x_{j,M}, u_{k,N}) + R_{M,2}(u_{k,N})\Big) + \int_{-1}^{1} R_{N,1}(x)\,dx. \tag{2.9}$$

Now equation (2.9) contains the expression $\sum_{k=1}^{N}\lambda_{k,N}R_{M,2}(u_{k,N})$ but, from equations (2.5) and (2.6), we have

$$\sum_{k=1}^{N}\lambda_{k,N}R_{M,2}(u_{k,N}) = \int_{-1}^{1} R_{M,2}(x)\,dx - \frac{1}{2\pi i}\int_{C_w} k_N(w) R_{M,2}(w)\,dw, \tag{2.10}$$

on assuming that the remainder $R_{M,2}(u)$ may be continued into the complex $w$-plane. In any case, the last term in (2.10) is essentially the "remainder of a remainder" and henceforth we shall assume that it is negligible and will replace it by zero. On combining (2.9) and (2.10) we find that

$$I \approx Q_{M,N} + \int_{-1}^{1} R_{N,1}(x)\,dx + \int_{-1}^{1} R_{M,2}(u)\,du, \tag{2.11}$$

where the quadrature sum $Q_{M,N}$ is given by

$$Q_{M,N} := \sum_{j=1}^{M}\sum_{k=1}^{N} \lambda_{j,M}\lambda_{k,N} f(x_{j,M}, u_{k,N}). \tag{2.12}$$

The remainder, or truncation error, $R_{M,N}$ for this quadrature sum is then approximated by

$$R_{M,N} := \int_{-1}^{1} R_{M,2}(u)\,du + \int_{-1}^{1} R_{N,1}(x)\,dx. \tag{2.13}$$

The question now arises as to how well this estimate of the error works out in practice and whether it can be used to obtain good asymptotic estimates of the quadrature error, on assuming that $M$ and $N$ are "large." The ability to obtain one significant digit accuracy for the estimate of the remainder will be useful in determining *a priori* the values of $M$ and $N$ to be used in any given case. We might note from [10] on assuming both $n$ "large" and $z$ bounded away from the interval $[-1, 1]$, that the function $k_n$ of (2.3) is given approximately by $\hat{k}_n(z)$ where

$$\hat{k}_n(z) := \frac{c_n}{(z + \sqrt{z^2 - 1})^{2n+1}}, \tag{2.14}$$

with

$$c_n := \frac{2\pi(\Gamma(n+1))^2}{\Gamma(n+1/2)\Gamma(n+3/2)}. \tag{2.15}$$

In the next two sections we shall consider, in detail, two examples. In §3 we shall consider the integral of (1.1) with $\alpha = 1$ so that the integrand, when continued into either the complex $z$-plane or complex $w$-plane, has simple poles. In §4 we shall choose $\alpha = 1/2$ so that, in this case, the integrand has branch point singularities in either of the complex planes. In each case we shall compare asymptotic estimates of the truncation error with the actual computed error and, in particular, consider how the accuracy of these estimates depends upon the parameter $b$.

## 3. An example with simple poles

We shall now consider the integral $I(a, b)$ defined by

$$I(a, b) := \int_{-1}^{1}\int_{-1}^{1} \frac{dx\,du}{(x-a)^2 + u^2 + b^2}, \tag{3.1}$$

where $-1 \le a \le 1$ and $b > 0$. Unfortunately, in this case we do not have an analytic expression for $I(a, b)$ although we have been able to calculate its value, for given values of $a$ and $b$, with considerable precision using a *Mathematica* (`www.wolfram.com`) program.

First, let us consider $R_{N,1}(x)$ where, from (2.6), we will have

$$R_{N,1}(x) = \frac{1}{2\pi i}\int_{C_w} \frac{k_N(w)\,dw}{w^2 + \big((x-a)^2 + b^2\big)}. \tag{3.2}$$

The integrand has simple poles at points $w_0$, $\overline{w}_0$ say, where

$$w_0 := ic \qquad \text{with} \qquad c := \sqrt{(x-a)^2 + b^2} > 0. \tag{3.3}$$

On letting the contour $C_w$ tend to infinity we find that

$$R_{N,1}(x) = -2\Re\{\operatorname*{res}_{w=ic} \frac{k_N(w)}{w^2 + \big((x-a)^2 + b^2\big)}\} \tag{3.4}$$

where $\operatorname*{res}_{w=ic}$ denotes the residue of the integrand at the point $w_0 = ic$. We have simply

$$\operatorname*{res}_{w=ic} \frac{k_N(w)}{w^2 + \big((x-a)^2 + b^2\big)} = \lim_{w\to ic} \frac{(w-ic)k_N(w)}{(w-ic)(w+ic)} = \frac{k_N(ic)}{2ic}. \tag{3.5}$$

From (2.14)

$$k_N(ic) \approx \hat{k}_N(ic) = \frac{c_N(-1)^N}{i(c+\sqrt{c^2+1})^{2N+1}}, \tag{3.6}$$

so that, from (3.4) - (3.6), we find

$$R_{N,1}(x) \approx \frac{c_N(-1)^N}{\sqrt{(x-a)^2+b^2}\Big(\sqrt{(x-a)^2+b^2} + \sqrt{(x-a)^2+b^2+1}\Big)^{2N+1}}. \tag{3.7}$$

In order to evaluate $\int_{-1}^{1} R_{N,1}(x)\,dx$ let us write

$$\sqrt{(x-a)^2+b^2} = \sinh(\theta+\theta_0), \tag{3.8}$$

with $x = a$ corresponding to $\theta = 0$ so that

$$b = \sinh\theta_0 \qquad \text{and} \qquad \cosh\theta_0 = \sqrt{1+b^2}. \tag{3.9}$$

Then

$$\sqrt{(x-a)^2+b^2} + \sqrt{(x-a)^2+b^2+1} = e^{\theta+\theta_0}, \tag{3.10}$$

where, from (3.9), we see that

$$e^{\theta_0} = b + \sqrt{1+b^2}. \tag{3.11}$$

Now, from (3.8),

$$\frac{(x-a)\,dx}{\sqrt{(x-a)^2+b^2}} = \cosh(\theta+\theta_0)\,d\theta. \tag{3.12}$$

But

$$(x-a)^2 = \sinh^2(\theta_0+\theta) - \sinh^2\theta_0 = \sinh(2\theta_0+\theta)\,\sinh\theta. \tag{3.13}$$

For $a \le x \le 1$ we shall write

$$(x-a) = \sqrt{\sinh(2\theta_0+\theta)\,\sinh\theta}, \tag{3.14}$$

but, for $-1 \le x \le a$, we have

$$(x-a) = -\sqrt{\sinh(2\theta_0+\theta)\,\sinh\theta}. \tag{3.15}$$

Again, from (3.8), let us define $\theta(-1)$ and $\theta(1)$ through

$$\sqrt{(1-a)^2+b^2} = \sinh(\theta(1)+\theta_0) \quad \text{and} \quad \sqrt{(1+a)^2+b^2} = \sinh(\theta(-1)+\theta_0). \tag{3.16}$$

Putting these results together gives

$$\int_{-1}^{1} R_{N,1}(x)\,dx \approx \frac{c_N(-1)^N}{(b+\sqrt{1+b^2})^{2N+1}}\Big(\int_0^{\theta(1)} + \int_0^{\theta(-1)}\Big)\frac{e^{-(2N+1)\theta}\cosh(\theta_0+\theta)\,d\theta}{\sqrt{\sinh\theta\,\sinh(2\theta_0+\theta)}}. \tag{3.17}$$

We see that if we assume $N$ is "large," then the major contribution to each integral comes from the neighbourhood of $\theta = 0$. Consequently, if we replace $\cosh(\theta_0+\theta)$ by $\cosh\theta_0$, $\sinh(2\theta_0+\theta)$ by $\sinh 2\theta_0$ and $\sinh\theta$ by $\theta$ we find that

$$\int_{-1}^{1} R_{N,1}(x)\,dx \approx \frac{c_N(-1)^N\cosh\theta_0}{\sqrt{\sinh 2\theta_0}(b+\sqrt{1+b^2})^{2N+1}}\Big(\int_0^{\theta(1)} + \int_0^{\theta(-1)}\Big)\frac{e^{-(2N+1)\theta}}{\sqrt{\theta}}\,d\theta. \tag{3.18}$$

Since, for all $X > 0$

$$\int_0^X \frac{e^{-(2N+1)\theta}}{\sqrt{\theta}}\,d\theta = \sqrt{\frac{\pi}{2N+1}}\operatorname{erf}(\sqrt{(2N+1)X}), \tag{3.19}$$

where erf denotes the error function, it follows that

$$\int_{-1}^{1} R_{N,1}(x)\,dx \approx \frac{\sqrt{\pi}(-1)^N c_N(1+b^2)^{1/4}}{\sqrt{2b(2N+1)}(b+\sqrt{1+b^2})^{2N+1}}\Big(\operatorname{erf}(\sqrt{(2N+1)\theta(1)})+\operatorname{erf}(\sqrt{(2N+1)\theta(-1)})\Big). \tag{3.20}$$

We might note that since we are assuming that $a$ and $b$ are real then it follows from (3.9), (3.16) and Abramowitz and Stegun [11, §4.6.20] that we can write

$$\theta(1) = \log\Big(\frac{\sqrt{(1-a)^2+b^2}+\sqrt{(1-a)^2+b^2+1}}{b+\sqrt{1+b^2}}\Big), \tag{3.21}$$

$$\theta(-1) = \log\Big(\frac{\sqrt{(1+a)^2+b^2}+\sqrt{(1+a)^2+b^2+1}}{b+\sqrt{1+b^2}}\Big).$$

So much for the second term of the remainder $R_{M,N}$ (see (2.13)). It now remains to consider the other term $\int_{-1}^{1} R_{M,2}(u)\,du$ where, from (2.8),

$$R_{M,2}(u) := \frac{1}{2\pi i}\int_{C_z} \frac{k_M(z)\,dz}{(z-a)^2+u^2+b^2}. \tag{3.22}$$

The integrand has simple poles at $z_0, \overline{z}_0$ where

$$z_0 := a + id \qquad \text{with} \qquad d := \sqrt{u^2+b^2}. \tag{3.23}$$

Arguing as before we have

$$R_{M,2}(u) = -2\Re\Big\{\operatorname*{res}_{z=a+id} \frac{k_M(z)}{\big((z-a)^2+u^2+b^2\big)}\Big\}. \tag{3.24}$$

We find

$$R_{M,2}(u) = \Re\Big\{\frac{ik_M(a+i\sqrt{u^2+b^2})}{\sqrt{u^2+b^2}}\Big\}. \tag{3.25}$$

From (2.14) we obtain

$$k_M(a+i\sqrt{u^2+b^2}) \approx \hat{k}_M(a+i\sqrt{u^2+b^2}) = \frac{c_M(-1)^M}{i\Big((\sqrt{u^2+b^2}-ia)+\sqrt{(\sqrt{u^2+b^2}-ia)^2+1}\Big)^{2M+1}} \tag{3.26}$$

so that

$$R_{M,2}(u) \approx c_M(-1)^M\Re\Big\{\frac{1}{\sqrt{u^2+b^2}\Big((\sqrt{u^2+b^2}-ia)+\sqrt{(\sqrt{u^2+b^2}-ia)^2+1}\Big)^{2M+1}}\Big\}. \tag{3.27}$$

In order to evaluate $\int_{-1}^{1} R_{M,2}(u)\,du = 2\int_0^1 R_{M,2}(u)\,du$, since $R_{M,2}$ is an even function, we write

$$\sqrt{u^2+b^2} - ia = \sinh(\phi+\phi_0) \tag{3.28}$$

with $u=0$ corresponding to $\phi=0$ so that

$$\sinh\phi_0 = b - ia \qquad \text{and} \qquad \cosh\phi_0 = \sqrt{1+(b-ia)^2}. \tag{3.29}$$

We also have

$$(\sqrt{u^2+b^2}-ia)+\sqrt{(\sqrt{u^2+b^2}-ia)^2+1} = e^{\phi+\phi_0} \tag{3.30}$$

where, from (3.29),

$$e^{\phi_0} = (b-ia)+\sqrt{1+(b-ia)^2}. \tag{3.31}$$

From (3.28) it follows that

$$\frac{u\,du}{\sqrt{u^2+b^2}} = \cosh(\phi+\phi_0)\,d\phi. \tag{3.32}$$

From (3.28) and (3.29) we have

$$\begin{aligned} u^2 =& \big(\sinh(\phi+\phi_0)+ia\big)^2 - b^2 \\ =& \big(\sinh(\phi+\phi_0)-\sinh\phi_0\big)\big(\sinh(\phi+\phi_0)+\sinh\overline{\phi}_0\big) \\ =& 4\cosh(\phi_0+\phi/2)\sinh(\phi/2)\sinh((\phi+\phi_0+\overline{\phi}_0)/2)\cosh((\phi+\phi_0-\overline{\phi}_0)/2). \end{aligned} \tag{3.33}$$

Since, as before, the major contribution to the integral when $M$ is "large" comes from the neighbourhood of $\phi = 0$ we shall, in (3.33) assume that $\phi$ is small so that we have approximately

$$\begin{aligned} u^2 \approx& \phi\cosh\phi_0 \times (2\sinh((\phi_0+\overline{\phi}_0)/2)\cosh((\phi_0-\overline{\phi}_0)/2)) \\ =& \phi\cosh\phi_0(\sinh\phi_0+\sinh\overline{\phi}_0), \end{aligned} \tag{3.34}$$

see Abramowitz and Stegun [11, §4.5.41]. Consequently

$$\begin{aligned} u^2 \approx& \phi\cosh\phi_0 \times 2\Re\{b-ia\}, \qquad \text{from (3.29)}, \\ =& 2b\phi\sqrt{1+(b-ia)^2}. \end{aligned} \tag{3.35}$$

From (3.32) and (3.35) we have

$$\frac{du}{\sqrt{u^2+b^2}} \approx \frac{(1+(b-ia)^2)^{1/4}\,d\phi}{\sqrt{2b\phi}} \tag{3.36}$$

so that, on putting this together, we find

$$\int_{-1}^{1} R_{M,2}(u)\,du \approx \frac{\sqrt{2}c_M(-1)^M}{\sqrt{b}}\Re\Big\{\frac{(1+(b-ia)^2)^{1/4}}{((b-ia)+\sqrt{(b-ia)^2+1})^{2M+1}}\int_0^{\phi_1}\frac{e^{-(2M+1)\phi}}{\sqrt{\phi}}\,d\phi\Big\}. \tag{3.37}$$

From (3.28), we have

$$\sqrt{1+b^2} - ia = \sinh(\phi_1+\phi_0) \tag{3.38}$$

and, from (3.29), it follows that

$$\phi_1 = \operatorname{arcsinh}(\sqrt{1+b^2}-ia) - \operatorname{arcsinh}(b-ia). \tag{3.39}$$

On recalling (3.19) we obtain our required result that

$$\int_{-1}^{1} R_{M,2}(u)\,du \approx \frac{\sqrt{2\pi}c_M(-1)^M}{\sqrt{b}\sqrt{2M+1}}\Re\Big\{\frac{(1+(b-ia)^2)^{1/4}\operatorname{erf}(\sqrt{(2M+1)\phi_1})}{((b-ia)+\sqrt{(b-ia)^2+1})^{2M+1}}\Big\}. \tag{3.40}$$

By combining (3.20) and (3.40) we now have an explicit estimate for $R_{M,N}$ assuming that $M$ and $N$ are "large". However, in practice, it turns out that since we are interested only in at most the first two significant digits in the remainder we can replace the values of the error function in both (3.20) and (3.40) by the value 1 to give, as our asymptotic estimate,

$$R_{M,N} \approx \frac{\sqrt{2\pi}(-1)^N c_N (1+b^2)^{1/4}}{\sqrt{b}\sqrt{2N+1}(b+\sqrt{1+b^2})^{2N+1}} + \frac{\sqrt{2\pi}(-1)^M c_M}{\sqrt{b}\sqrt{2M+1}} \Re\Big\{ \frac{(1+(b-ia)^2)^{1/4}}{((b-ia)+\sqrt{(b-ia)^2+1})^{2M+1}} \Big\}. \tag{3.41}$$

In Table 3.1 we have considered an example in which we have chosen $M = 20$, $N = 15$, fixed $a$ at $1/4$ and considered various values of $b$.

| | $b = 1/2$ | $b = 1/5$ | $b = 1/10$ | $b = 1/20$ | $b = 1/30$ |
|---|---|---|---|---|---|
| actual error | $-1.40 \times 10^{-6}$ | -0.0144 | -0.523 | -4.70 | -11.20 |
| equation (3.41) | $-1.39 \times 10^{-6}$ | -0.0142 | -0.471 | -3.43 | -7.35 |

Table 3.1: $M = 20, N = 15, a = 1/4$

As can be seen, for $b = 1/2, 1/5$ and $1/10$ the asymptotic estimate of the error agrees with the actual error to at least one significant digit. However, as $b$ becomes smaller so the accuracy of the estimate diminishes although even for $b = 1/30$ the sign is correct! When $b$ is small the singularity of the integrand is very close to the region of integration in the $(x, u)$ plane and it is suggested that for such $b$ the estimate of $k_n$ as given in (2.14) is not good enough. The investigation of this is beyond the scope of this paper.

Table 3.2 shows a similar comparison with $b$ fixed at $1/10$ and the number of integration points increasing (with the restriction that $M = N$). The Table shows that as $N$ increases, not

| | $M = N = 10$ | $M = N = 15$ | $M = N = 20$ | $M = N = 25$ | $M = N = 30$ |
|---|---|---|---|---|---|
| actual error | $+1.11$ | $-7.84 \times 10^{-2}$ | $+9.55 \times 10^{-2}$ | $-4.67 \times 10^{-2}$ | $+1.84 \times 10^{-2}$ |
| equation (3.41) | $+1.21$ | $-1.82 \times 10^{-1}$ | $+7.97 \times 10^{-2}$ | $-4.67 \times 10^{-2}$ | $+1.95 \times 10^{-2}$ |

Table 3.2: $M = N$, $a = 1/2$, $b = 1/10$

only does the actual error decrease, as would be expected, but also equation (3.41) becomes a better approximation to the actual error. Such a result is to be expected as the approximation suggested in equation (2.14) improves with increasing $N$.

We shall now turn our attention to the second example where the integrand has branch point singularities.

## 4. An example with branch point singularities

Let us consider the integral $I(b)$ where

$$I(b) := \int_{-1}^{1} \int_{-1}^{1} \frac{dx\, du}{\sqrt{x^2 + u^2 + b^2}}, \tag{4.1}$$

and $b > 0$. In this case we have an analytic expression for the integral, so that

$$I(b) = 4 \log \Big( \frac{\sqrt{2 + b^2} + 1}{\sqrt{2 + b^2} - 1} \Big) - 4b \arctan \Big( \frac{1}{b\sqrt{2 + b^2}} \Big). \tag{4.2}$$

Since the integrand is a symmetric function in $x$ and $u$ we shall, throughout this section, assume that $M = N$. Consequently we have from (2.6) and (2.8) that $R_{N,2}(u) = R_{N,1}(u)$ so that, from (2.13), the remainder $R_{N,N}$ is given by

$$R_{N,N} = 2 \int_{-1}^{1} R_{N,2}(u)\, du. \tag{4.3}$$

But, since

$$R_{N,2}(u) = \frac{1}{2\pi i} \int_{C_z} \frac{k_N(z)\, dz}{\sqrt{z^2 + u^2 + b^2}}, \tag{4.4}$$

we see that $R_{N,2}(u)$ is an even function of $u$ so that, from (4.3), we have

$$R_{N,N} = 4 \int_{0}^{1} R_{N,2}(u)\, du. \tag{4.5}$$

To evaluate the contour integral in (4.4), if we write

$$c := \sqrt{u^2 + b^2}, \qquad \text{with} \qquad c > 0, \tag{4.6}$$

then the integrand has branch points at $z_0, \overline{z}_0$ where

$$z_0 := ic. \tag{4.7}$$

On letting the contour $C_z$ go to infinity then we have, see Figure 1, that

$$R_{N,2}(u) = 2\Re\Big\{ \frac{1}{2\pi i} \int_{AB \cup CD} \frac{k_N(z)\, dz}{\sqrt{z^2 + c^2}} \Big\}. \tag{4.8}$$

Now along $AB$ we have $z - ic = re^{i\pi/2}$ with $r$ going from $\infty$ to 0. Along $CD$, we have $z - ic = re^{-3\pi i/2}$ with $r$ going from 0 to $\infty$. From (4.8) it can be shown that

$$R_{N,2}(u) = \frac{2}{\pi}\Re\Big\{e^{i\pi/2}\int_0^\infty \frac{k_N((r+c)e^{i\pi/2})\,dr}{\sqrt{r}\sqrt{r+2c}}\Big\}. \tag{4.9}$$

With $\hat{k}_N$ as defined in (2.14) we obtain

$$R_{N,2}(u) \approx \frac{2(-1)^N c_N}{\pi}\int_0^\infty \frac{dr}{\sqrt{r}\sqrt{r+2c}\big((r+c)+\sqrt{(r+c)^2+1}\big)^{2N+1}}. \tag{4.10}$$

In order to evaluate this integral let us write

$$r + c = \sinh(\theta + \theta_0), \tag{4.11}$$

with $r = 0$ corresponding to $\theta = 0$ so that

$$c = \sinh\theta_0 \qquad \text{and} \qquad \cosh\theta_0 = \sqrt{1+c^2}. \tag{4.12}$$

From (4.11) we have $dr = \cosh(\theta + \theta_0)\,d\theta$ and, from (4.11) and (4.12), we find that

$$r = 2\sinh(\theta/2)\cosh(\theta_0 + \theta/2) \quad \text{and} \quad r + 2c = 2\cosh(\theta/2)\sinh(\theta_0 + \theta/2). \tag{4.13}$$

Finally, we note that

$$(r+c) + \sqrt{(r+c)^2+1} = e^{\theta+\theta_0} \tag{4.14}$$

where, from (4.12), it follows that

$$e^{\theta_0} = c + \sqrt{1+c^2}. \tag{4.15}$$

Combining (4.10) - (4.15) we obtain

$$R_{N,2}(u) \approx \frac{2(-1)^N c_N}{\pi(c+\sqrt{1+c^2})^{(2N+1)}}\int_0^\infty \frac{e^{-(2N+1)\theta}\cosh(\theta_0+\theta)\,d\theta}{\sqrt{\sinh\theta}\sqrt{\sinh(2\theta_0+\theta)}}. \tag{4.16}$$

Now the integrand of this integral is exactly the same as that discussed in the previous section at equation (3.17). Since the main contribution to the integral comes from the neighbourhood of $\theta = 0$ then making the same assumptions as before and recalling from (3.19), that

$$\int_0^\infty \theta^{-1/2}e^{-(2N+1)\theta}\,d\theta = \sqrt{\pi}/\sqrt{2N+1}, \tag{4.17}$$

we find that(4.16) gives

$$R_{N,2}(u) \approx \frac{\sqrt{2}(-1)^N c_N (u^2+1+b^2)^{1/4}}{\sqrt{(2N+1)\pi}(u^2+b^2)^{1/4}(\sqrt{u^2+b^2}+\sqrt{u^2+1+b^2})^{2N+1}}. \tag{4.18}$$

From (4.5) and (4.18) we have that

$$R_{N,N} \approx \frac{4\sqrt{2}(-1)^N c_N}{\sqrt{\pi}\sqrt{2N+1}} J_N(b) \tag{4.19}$$

say, where the integral $J_N(b)$ is defined by

$$J_N(b) := \int_0^1 \frac{(u^2+1+b^2)^{1/4}\,du}{(u^2+b^2)^{1/4}(\sqrt{u^2+b^2}+\sqrt{u^2+1+b^2})^{2N+1}}. \tag{4.20}$$

In order to evaluate this integral we make a similar transformation to that in (3.28) by writing

$$\sqrt{u^2+b^2} = \sinh(\phi+\phi_0) \tag{4.21}$$

with $u = 0$ corresponding to $\phi = 0$ so that we have

$$b = \sinh\phi_0 \qquad \text{and} \qquad \cosh\phi_0 = \sqrt{1+b^2}. \tag{4.22}$$

It follows that

$$\sqrt{u^2+b^2} + \sqrt{u^2+1+b^2} = e^{\phi+\phi_0} \tag{4.23}$$

where, from (4.22), we have

$$e^{\phi_0} = b + \sqrt{1+b^2}. \tag{4.24}$$

From (4.21)

$$u\,du = \sinh(\phi+\phi_0)\cosh(\phi+\phi_0)\,d\phi, \tag{4.25}$$

and, from (4.21) and (4.22), we obtain

$$u = \sqrt{\sinh\phi\,\sinh(2\phi_0+\phi)}. \tag{4.26}$$

Combining (4.20) - (4.26) gives

$$J_N(b) = \frac{1}{(b+\sqrt{1+b^2})^{2N+1}} \int_0^{\phi_1} \frac{e^{-(2N+1)\phi}\sqrt{\sinh(\phi_0+\phi)}(\cosh(\phi_0+\phi))^{3/2}\,d\phi}{\sqrt{\sinh\phi}\sqrt{\sinh(2\phi_0+\phi)}}, \tag{4.27}$$

where $\phi_1$ is such that

$$\phi_1 = \operatorname{arcsinh}\sqrt{1+b^2} - \operatorname{arcsinh} b = \log\Big(\frac{\sqrt{1+b^2}+\sqrt{2+b^2}}{b+\sqrt{1+b^2}}\Big). \tag{4.28}$$

Again, we see that for $N$ "large", the major contribution to the integral comes from the neighbourhood of $\phi = 0$. On replacing $\sinh(\phi_0+\phi)$ by $\sinh\phi_0$, $\cosh(\phi_0+\phi)$ by $\cosh\phi_0$, $\sinh(2\phi_0+\phi)$ by $\sinh(2\phi_0)$ and $\sinh\phi$ by $\phi$ we have

$$\begin{aligned} J_N(b) &\approx \frac{\sqrt{1+b^2}}{\sqrt{2}(b+\sqrt{1+b^2})^{2N+1}} \int_0^{\phi_1} e^{-(2N+1)\phi}\phi^{-1/2}\,d\phi \qquad (4.29)\\ &= \frac{\sqrt{\pi}\sqrt{1+b^2}\,\operatorname{erf}(\sqrt{(2N+1)\phi_1})}{\sqrt{2}\sqrt{2N+1}(b+\sqrt{1+b^2})^{2N+1}}, \end{aligned}$$

on recalling (3.19). On combining (4.19) with (4.29) we obtain our required result that

$$R_{N,N} \approx \frac{4(-1)^N c_N \sqrt{1+b^2}\, \mathrm{erf}(\sqrt{(2N+1)\phi_1})}{(2N+1)(b+\sqrt{1+b^2})^{2N+1}}. \tag{4.30}$$

Let us see how good this estimate of the error is, by considering some numerical examples. Firstly, with $b = 1/2$ we find in Table 4.1 the following comparison of exact errors with the asymptotic estimates of (4.30) for $N = 10(5)25$.

| $N$ | actual error | equation (4.30) |
|---|---|---|
| 10 | $+5.49 \times 10^{-5}$ | $+5.34 \times 10^{-5}$ |
| 15 | $-3.04 \times 10^{-7}$ | $-2.96 \times 10^{-7}$ |
| 20 | $+1.86 \times 10^{-9}$ | $+1.83 \times 10^{-9}$ |
| 25 | $-1.22 \times 10^{-11}$ | $-1.20 \times 10^{-11}$ |

Table 4.1: $b = 1/2$

We see from Table 4.1 that the asymptotic estimate of $R_{N,N}$ as given by (4.30) gives almost two significant digits of the actual error. However, as in §3, the estimate of error deteriorates as we let $b$ become smaller. In Table 4.2 we have chosen $N = 20$ and compared the exact error with the asymptotic estimate for decreasing $b$.

| | $b = 1/5$ | $b = 1/10$ | $b = 1/20$ | $b = 1/30$ | $b = 1/40$ |
|---|---|---|---|---|---|
| actual error | $+1.78 \times 10^{-4}$ | $+8.95 \times 10^{-3}$ | $+5.52 \times 10^{-2}$ | $+9.55 \times 10^{-2}$ | $+1.24 \times 10^{-1}$ |
| equation (4.30) | $+1.79 \times 10^{-4}$ | $+1.02 \times 10^{-2}$ | $+7.81 \times 10^{-2}$ | $+1.55 \times 10^{-1}$ | $+2.17 \times 10^{-1}$ |

Table 4.2: $N = 20$

As can be seen, the asymptotic estimate becomes worse as $b$ tends to zero. It might be noted in passing that we get precisely the same asymptotic estimates in Tables 4.1 and 4.2 if, in equation (4.30), we replace $\mathrm{erf}(\sqrt{(2N+1)\phi_1})$ by 1.

## 5. Conclusion

In this paper we have considered the truncation error when Gauss-Legendre quadrature is used to evaluate double integrals taken over the region $(-1,1) \times (-1,1)$. There appears to be no literature on this specific topic so we have first derived an approximate expression for this truncation error, see equation (2.13). This expression is given in terms of contour integrals since we have assumed that the definition of the integrand can be continued into the appropriate complex planes. Such will be the case for the sort of integrals envisaged here which arise from the boundary integral method.

By approximating these contour integrals we have then considered asymptotic estimates of the remainder in two important cases. In the first example we have assumed that the singularities of the integrand are poles and, in the second example, that they are branch points. It appears that, provided the singular point of the integrand is not too close to the surface $(-1,1) \times (-1,1)$, these asymptotic estimates are quite good, giving one or two correct significant digits.

In the context of the boundary integral method, the authors, in [7] and [8] have advocated the use of the sinh- and iterated sinh- transformations in order to give greater accuracy for a given number of quadrature points. However, we have not considered the effects of these transformations on the integrals discussed here, but will leave such results for a future paper, or two.

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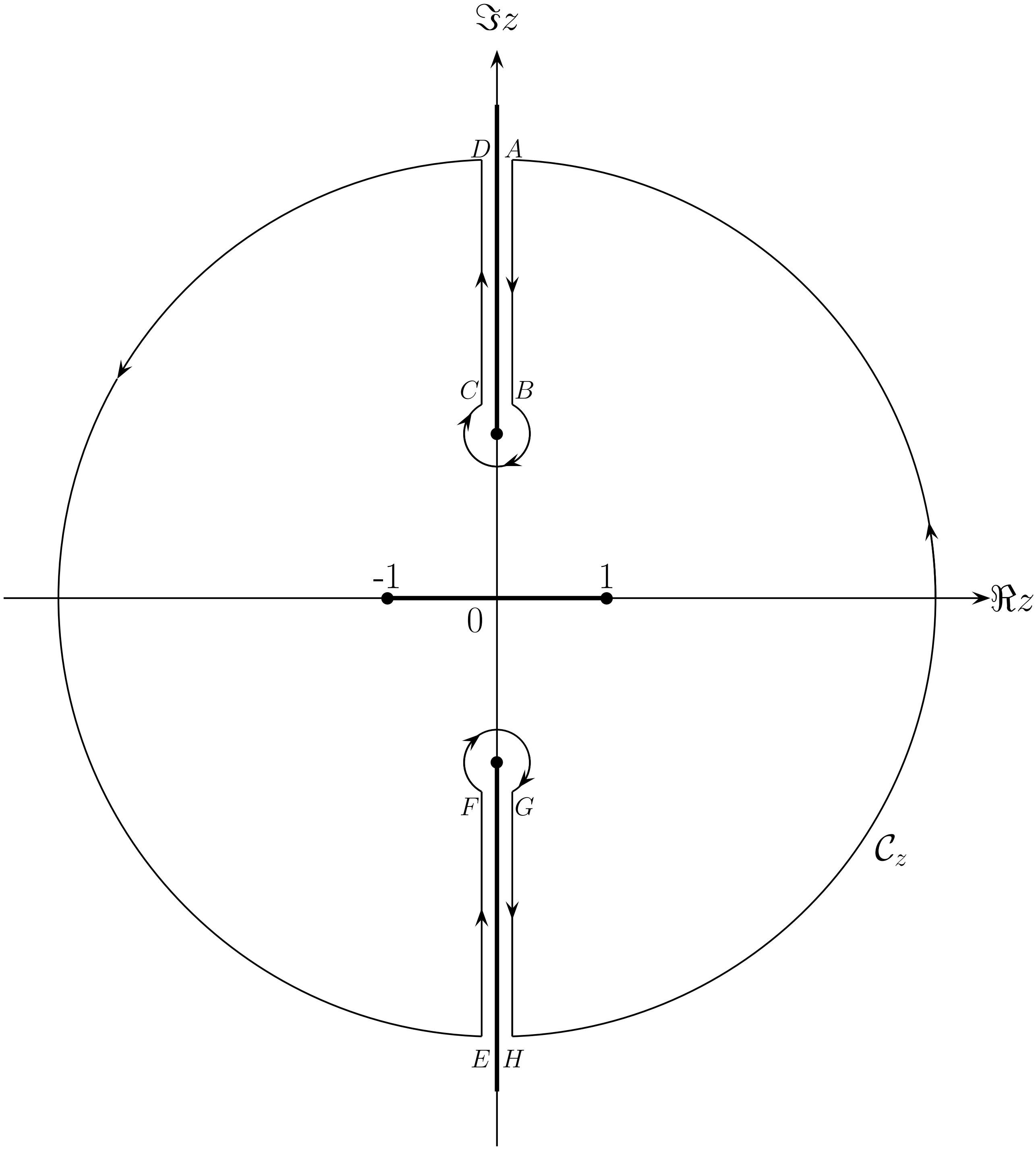


Figure 1: Contour for the evaluation of the integral (4.4)