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A comparison of the error function and the tanh transformation as progressive rules for double and triple singular integrals

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Abstract: Transformations of the form $x = \tanh(g(t))$ for $g(t) = t^n$ and for $g(t) = c \sinh(t)$, as well as transformations of the error function type are employed on double and triple singular integrals. Extensions of the one-dimensional approach allow variable limit multiple integrals to be attempted successfully. Some shortcomings of the double exponential or DE rule are exposed in the comparisons. Finally, comparison is made with the method of good lattice points (Sugihara, 1987).

Keywords: Singular multiple quadrature, singular double integrals, singular triple integrals.

1. Introduction

The transformation

$$x = \tanh(t^n)$$

has been studied extensively for handling one-dimensional singular integrals by Takahasi and Mori [8], Mori [5,6] and Evans, Forbes and Hyslop [4]. The higher derivatives of the function vanish exponentially at $\pm\infty$ allowing the trapezium rule to behave as a very high order technique, and at the same time the singularity is removed.

More recently Aihie and Evans [1] extended this technique to two dimensions by considering integrals of the form

$$I = \int_{-1}^{1}\int_{-1}^{1} f(x, y)\, \mathrm{d}x\, \mathrm{d}y, \tag{1}$$

where a linear transformation is employed to reduce any general finite range to $(-1, 1)$.

By setting $x = \tanh \alpha^n$ and $y = \tanh \beta^n$, (1) becomes

$$I = n^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\tanh \alpha^n, \tanh \beta^n)(\alpha\beta)^{n-1} \operatorname{sech}^2\alpha^n \operatorname{sech}^2\beta^n\, \mathrm{d}\alpha\, \mathrm{d}\beta. \tag{2}$$

Two strategies were then adopted in implementing (2). First a further transformation was initiated by making the substitution

$$\alpha = r\cos\theta \quad \text{and} \quad \beta = r\sin\theta,$$

in (2) so yielding

$$I = r^2 \int_0^{\infty} \int_0^{2\pi} G(r\cos\theta,\ r\sin\theta) r\,\mathrm{d}r\,\mathrm{d}\theta, \tag{3}$$

where

$$G(\alpha,\beta) = g(\alpha,\beta)(\alpha\beta)^{n-1}\operatorname{sech}^2\alpha^n \operatorname{sech}^2\beta^n,$$

and

$$g(\alpha,\beta) = f(\tanh\alpha^n,\ \tanh\beta^n).$$

The trapezoidal rule was applied to (3) to give

$$I = n^2h^2 \sum_{i=0}^{m} i \int_0^{2\pi} G(ih\cos\theta,\ ih\sin\theta)\,\mathrm{d}\theta. \tag{4}$$

Clenshaw–Curtis quadrature was then used to complete the evaluation of (4) from 0 to 2π. The total effect of this was that integration was carried out in concentric circles until further contributions to the quadrature were insignificant.

The other strategy was to invoke the trapezoidal rule in both dimensions. Hence (2) was evaluated as

$$I = 4n^2h_1h_2 \sum_i \sum_j f(\tanh\alpha_i^n,\ \tanh\beta_j^m)(\alpha_i\beta_j)^{n-1}\operatorname{sech}^2\alpha_i^n \operatorname{sech}^2\beta_j^n, \tag{5}$$

where α_i and β_j are the trapezoidal rule points and i and j cover the region of significant contributions to the quadrature. In implementing (5) it was necessary to set up a grid in the infinite plane whose boundary was determined by the monitoring of the values of the integrand.

By exactly the same philosphy the error function transformation can also be implemented. Here instead of the tanh transformation in (1) we adopt the substitutions

$$x = g(t) \quad \text{and} \quad y = g(u), \tag{6}$$

where

$$g(t) = c\int_0^t \mathrm{e}^{-u^{2n}}\,\mathrm{d}u.$$

As demonstrated by Aihie and Evans [2], $g(t)$ maps the interval $(-1, 1)$ into $(-\infty, \infty)$; hence (1) becomes

$$I = c^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(g(t),\ g(u))\ \mathrm{e}^{-t^{2n}}\ \mathrm{e}^{-u^{2n}}\,\mathrm{d}t\,\mathrm{d}u. \tag{7}$$

As in (3), if we adopt the substitution

$$t = r\cos\theta \quad \text{and} \quad u = r\sin\theta, \tag{8}$$

we have

$$I = c^2 \int_0^{2\pi} \int_0^{\infty} f(g(r\cos\theta),\ g(r\sin\theta))\ \mathrm{e}^{(r\cos\theta)^{2n}}\ \mathrm{e}^{-(r\sin\theta)^{2n}}\ r\,\mathrm{d}r\,\mathrm{d}\theta. \tag{9}$$

Now putting

$$f(g(t),\ g(u)) = b(t,\ u) \quad \text{and} \quad B(t,\ u) = b(t,\ u)\ \mathrm{e}^{-t^{2n}}\mathrm{e}^{-u^{2n}},$$

reduces equation (9) to

$$I = c^2 \int_0^{2\pi} \int_0^{\infty} B(r \cos \theta,\ r \sin \theta) r \,\mathrm{d}r \,\mathrm{d}\theta, \tag{10}$$

so allowing either strategy to be employed.

Finally the double exponential or DE transformation defined by

$$x = \tanh(c \sinh \alpha) \tag{11}$$

and

$$y = \tanh(c \sinh \alpha) \tag{12}$$

was employed with $c = 1$. This transformation is generally accepted as resulting in a quadrature rule with errors which are asymptotically smaller than the earlier transformations of equations (2) and (9) [6]. Hence the quadrature rule is now

$$\begin{aligned} I = 4c^2 h_1 h_2 \sum_i \sum_j f\big(\tanh(c \sinh \alpha_i),\ \tanh(c \sinh \beta_j)\big) \\ \times \operatorname{sech}^2(c \sinh \alpha_i) \operatorname{sech}^2(c \sinh \beta_j) \cosh(\alpha_i) \cosh(\beta_j), \end{aligned} \tag{13}$$

which corresponds to (5) for the simple $\tanh(t^n)$ transformation.

2. Extension to variable limits

In the preparation of this work the authors have been presented with some examples which have previously proved intractable. One such example is

$$\int_0^2 \int_0^4 \sqrt{20 - x^2 - y^2}\ \ln |y^2 - x| \,\mathrm{d}x \,\mathrm{d}y. \tag{14}$$

Here the singularities lie inside the region of integration and it is natural to evaluate the integral in two parts, splitting the region at the boundary of discontinuity. This results in the two integrals

$$\int_0^2 \int_0^{y^2} \sqrt{20 - x^2 - y^2}\ \ln |y^2 - x| \,\mathrm{d}x \,\mathrm{d}y + \int_0^2 \int_{y^2}^4 \sqrt{20 - x^2 - y^2}\ \ln |y^2 - x| \,\mathrm{d}x \,\mathrm{d}y, \tag{15}$$

which requires a variable limit to be handled. This is achieved by the simple device, in terms of programming, of including a transformation of the local inner integration range for a current outer integration point to the standard range $(-1, 1)$. Hence a transformation of the form

$$x_2 = (b(y) - a(y)) \cdot \tfrac{1}{2} x_1 + \tfrac{1}{2}(b(y) + a(y)) \tag{16}$$

is used where the subprogramme parameters for the limits are now themselves functions of the outer integration range y. This code can be used without any marked loss of speed for the previous cases with singularities at fixed points. The results for these integrals are presented in Section 4.

3. Extension to three dimensions

The design of the code was so arranged to allow easy extension to higher dimensions. Again by analogy with two dimensions, two situations arise in halving the step size and re-using existing function values for a progressive rule. These are illustrated in Fig. 1.

The bold lines indicate the first set of points. Along these x-directions new intermediate points can be simply added in. This is the first situation. However subdivision in the y-direction will result in intermediate search directions with no existing points (the light lines). For these directions a search using the current step length is made to fix the relevant end-point for the new line. This is the second situation.

Clearly in three dimensions, a two-dimensional search is required in the equivalent situation to fix a whole plane of new intermediate points for a given new intermediate z-value. The above two-dimensional procedure is also required to complete the addition of points to the planes with the original z-values. This is a clear case of recursion from a computational point of view in which a search routine with dimension as a parameter can call itself as required. In practice, however, it is rare to require the same routine to perform for varying dimension. For the purpose of these tests a separate three-dimensional routine was used.

A further problem which arises with high dimensions is the high number of function evaluations needed to effect even a low accuracy quadrature. With singularities present efficient one-dimensional quadratures use the order of 30 points for 8 figure accuracy. A three-dimensional equivalent is of order 27,000. In fact this is an overestimate as often the singular part is handled in only one of the quadratures. However, if progression is used to confirm accuracy of an integral by step reduction, a halving of the step size in all dimensions yields an enormous function count at the second step. In the two-dimensional cases only one such subdivision was executed for this reason: in three dimensions even this could prove excessive.

Instead the search step was adjusted to allow a more accurate run to be made without having to halve the step size.

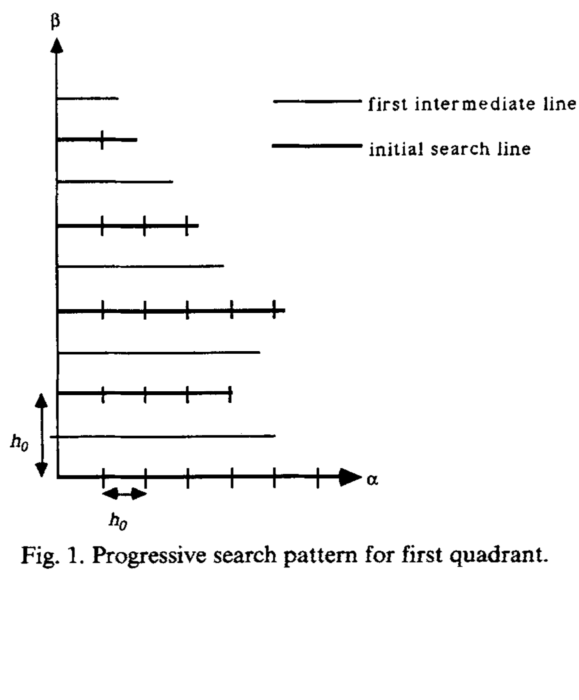

Fig. 1. Progressive search pattern for first quadrant.

Again the three-dimensional version used the variable limit implementation of Section 2, and both used the doubly infinite range strategy of (5). The possible criticism of the Clenshaw–Curtis and trapezoidal combination is that on the range $[0, \infty]$ the trapezoidal rule is not being used on an integrand with all its higher derivatives vanishing at the two end-points—the theoretical basis of the high accuracy obtained. Though this is the case at ∞, at 0 only the first few derivatives vanish because of the terms $(\alpha\beta)^{n-1}$ in (3) with $r\,\mathrm{d}r\,\mathrm{d}\theta$ gives a power r^{2n-1}. Hence in practice this approach is not obviously less good than the alternative of integrating r from $(-\infty, \infty)$ and then letting θ go from $(0, \pi)$.

At first sight it looks as though having all the higher derivative end-points to vanish is a laudable end. However such vanishing does not make the trapezoidal rule arbitrarily accurate. The reason is that the error term in the Euler–Maclaurin sum on which this work is based is an *asymptotic series*. An experiment was carried out with a well-behaved series of integrals using a Romberg-like approach to see at which term the error series terminated in practice. The results gave a quite low order cut off around order five—much in line with the findings above for the limit at zero. This is also why for nonsingular integrals such a method is not competitive with a straight application of Clenshaw–Curtis or Patterson.

All the examples use an integrand programmed as a function of two variables for each actual variable, being the distances from each end of the range of integration of the actual variable. This technique is discussed in [1] and a specific example is illustrated in the three-dimensional examples.

4. Tests and results

In Table 1, seven test integrals which have been considered in [1] are now evaluated with the error function transformation and the results compared with the original tanh form and the DE transformation. In making comparisons it must be remembered that for $n \neq 1$ the error function transformation is not a standard function and hence some extra effort is required to evaluate the transformation as discussed in [2].

Both the Clenshaw–Curtis trapezoidal rule combination and the trapezoidal product rule were implemented with the error function transformation. It was found that the error transformation yielded integrals which proved considerably less amenable to completion by Clenshaw–Curtis than the original tanh transformation. Hence for example on I_1 with 7738 points a value of 1.66624372 resulted, the errors arising from the inability of the Clenshaw–Curtis quadrature to handle the transformed integral.

As a product rule however the error function is competitive with tanh, though more involved to implement for $n > 1$. For integrals with singular integrands, the DE transform performs best of the group, but quite poor performance is observed on integrals I_6 and I_7 which have singularities in their first derivatives.

In Table 2, three examples which involve variable limits and hence curves of singularities were evaluated. The analytic values of these integrals are, in general, not known and hence a straight application of a Gauss–Legendre product rule was used as a reliable way of obtaining a low accuracy value. The tanh transformation and the DE rule were employed, as the gain in function evaluations in using the error function would seem to be outweighed by the extra work in evaluating the transformation $g(t)$ itself, the integrands being of a simple nature.

Table 1
Relative errors involved in evaluating the test integrals by tanh and error function transformations

Integrals	Analytic values	Clenshaw–Curtis and trapezoidal rule	Trapezoidal product rule					
		tanh	tanh			Error function		
			$n=3$	$n=5$	DE	$n=1$	$n=2$	$n=3$
$I_1=\int_0^1\int_0^1\frac{\mathrm{d}x\,\mathrm{d}y}{1-xy}$	$\frac{1}{6}\pi^2$	$-1.41(-5)$	$-4.56(-7)$	$-2.09(-6)$	$1.10(-6)$	$-2.17(-6)$	$-4.48(-7)$	$1.18(-6)$
	1.6449341	(3840)	(3597)	(1975)	(728)	(8420)	(3962)	(1728)
$I_2=\int_{-1}^1\int_{-1}^1\frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{1-x^2y^2}}$	$2\pi\ln 2$	$-1.20(-6)$	$-4.59(-9)$	$-9.41(-8)$	$-7.83(-8)$	$4.28(-10)$	$2.78(-8)$	$9.67(-8)$
	4.3551722	(3840)	(3653)	(1973)	(736)	(9200)	(3908)	(1728)
$I_3=\int_{-1}^1\int_{-1}^1\frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{2-x-y}}$	$\frac{16}{3}(2-\sqrt{2})$	$-3.10(-7)$	$-1.54(-7)$	$-4.80(-8)$	$-8.64(-8)$	$1.20(-6)$	$-2.51(-7)$	$-1.26(-7)$
	3.1241943	(3840)	(3535)	(1958)	(706)	(9200)	(3908)	(1718)
$I_4=\int_{-1}^1\int_{-1}^1\frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{3-x-2y}}$	$\frac{4}{3}\sqrt{2}[3\sqrt{3}-2\sqrt{2}-1]$	0.0	$-2.91(-7)$	$-1.98(-7)$	$-1.86(-7)$	$-9.09(-7)$	$-2.96(-7)$	$-2.50(-7)$
	2.5790076	(8153)	(3514)	(1956)	(589)	(9153)	(3903)	(1714)
$I_5=\int_0^1\int_0^1(xy)^{1/2}\,\mathrm{d}x\,\mathrm{d}y$	4.0	$1.16(-4)$	$-2.53(-7)$	$-1.80(-7)$	$-5.96(-8)$	$-1.37(-5)$	$2.12(-5)$	$-2.14(-5)$
		(6786)	(4532)	(3542)	(860)	(17570)	(8178)	(2817)
$I_6=\int_{-1}^1\int_{-1}^1\lvert x^2+y^2-\frac{1}{4}\rvert\,\mathrm{d}x\,\mathrm{d}y$	$\frac{5}{3}+\frac{1}{16}\pi$	$4.83(-8)$	$1.57(-7)$	$2.64(-7)$	$-1.37(-4)$	$2.11(-7)$	$3.18(-7)$	$-2.64(-7)$
	1.8630162	(2944)	(4453)	(1961)	(2712)	(11037)	(2993)	(1901)
$I_7=\int_0^1\int_0^1\lvert x-y\rvert^{1/2}\,\mathrm{d}x\,\mathrm{d}y$	$\frac{8}{15}$	$7.31(-8)$	$+8.77(-8)$	$+6.90(-8)$	$-3.92(-3)$	$5.02(-8)$	$6.90(-8)$	$8.77(-8)$
	0.5333333	(7119)	(3441)	(2751)	(6843)	(10887)	(3811)	(1689)

The figures in parentheses represent the number of function evaluations.

Table 2
Values for non end-point singular integrals

Integral	Gauss results	tanh rule			
		$n=3$	$n=3$	$n=5$	DE
$I_8=\int_0^1\int_0^1 \sin^{1/2}(xy)\ln\lvert x^3-y^3\rvert\,dx\,dy$	-0.706841938 *	-0.70682656	-0.70682640	-7.06826448	-0.70682654
	(256)	(739)	(2823)	(1669)	(536)
$I_9=\int_0^1\int_0^1\lvert x-y\rvert^{1/2}\,dx\,dy$	true value	0.5333333		0.5333333	0.5333333
	$\frac{8}{15}$	(740)		(1662)	(234)
$I_{10}=\int_0^2\int_0^4\sqrt{20-x^2-y^2}$	-2.38911408	-2.4420488	-2.4420485	-2.4420488	-2.4420486
$\times\ln\lvert y^2-x\rvert\,dx\,dy$	(256)	(843+895)	(3273+3427)	(1806+1891)	(620+662)

* Gauss–Legendre and a Gauss-ln formula were used here. The figures in parentheses represent the number of function evaluations.

Integrals I_8 and I_9 were evaluated as

$$2\int_0^1\int_0^y \sin^{1/2}(xy)\ \ln\lvert x^3-y^3\rvert\,dx\,dy \quad\text{and}\quad 2\int_0^1\int_0^y\lvert x-y\rvert^{1/2}\,dx\,dy \tag{17}$$

because of their symmetry about $x=y$, integral I_{10} was split into the two integrals shown in (15) and the function count for both halves is shown. Integral I_9 is now linear and is resolved to machine accuracy without recourse to further subdivision. The progressive subdivision yields good agreement in I_8 and I_{10}, demonstrating well the power of the method.

In Table 3 five three-dimensional singular integrals have been evaluated with the extended code. The analytic values of four of these integrals have been found and quoted for reference. In the case of example I_{14} a Gauss product rule was used as a means of obtaining a low accuracy value as a check against a mis-program occurring in the main code. The integral in I_{14} required splitting to ensure that the singularities were at the end-points of the dynamic range. Hence the integral I_{14} was written as

$$\begin{aligned}I_{14}&=\int_0^1\int_0^1\int_0^1\frac{\sin^{1/2}(xyz)}{(\lvert x+y-z\rvert)^{3/4}}\,dx\,dy\,dz\\&=\int_0^1\int_0^{1-x}\int_{x+y}^{1.0}\frac{\sin^{1/2}(xyz)}{(z-x-y)^{3/4}}\,dz\,dy\,dx+\int_0^1\int_0^{1-x}\int_0^{x+y}\frac{\sin^{1/2}(xyz)}{(x+y-z)^{3/4}}\,dz\,dy\,dx\\&\quad+\int_0^1\int_0^1\int_{1-x}^1\frac{\sin^{1/2}(xyz)}{(x+y-z)^{3/4}}\,dy\,dx\,dz=I_{141}+I_{142}+I_{143},\quad\text{say.}\end{aligned}\tag{18}$$

As in all the examples the integrand is programmed as a function of two variables for each actual variable giving six in three dimensions, i.e., $f(x_1, y_1, z_1, x_2, y_2, z_2)$ where x_1 is the distance of x from the lower end-point and x_2 is the distance from the upper end-point. Hence as in all the previous work cancellation in evaluating the integrand near the singularity is eliminated. Hence in I_{141} we have $z=x+y+z_1=1.0-z_2$, and so the denominator is coded as $(z_1)^{3/4}$. A further problem of cancellation can occur in variable limit examples and in I_{141} it is required to evaluate $1.0-x-y$ for the range of integration in the z-variable. Cancellation occurs when $x+y\sim 1.0$,

Table 3
Values for three-dimensional singular integrals

Integral	Analytic values	tanh product rule, $n=3$		DE rule
$I_{11}=\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{1-\cos x\cos y\cos z}$	$4\pi K^2(\frac{1}{2}\sqrt{2})=43.1980665$	43.198325	43.3234143	43.210988
		(78208)	(10722)	(77432)
$I_{12}=\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{3-g(x,y)-g(x,z)-g(y,z)}$	$\sqrt{3}\,\pi K^2(\sin\pi/12)=13.897646$	13.8976554	13.9288723	13.9019318
and $g(x,y)=\cos x\cos y$		(72848)	(10324)	(71032)
$I_{13}=\int_0^{\pi}\int_0^{\pi}\int_0^{\pi}\frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{3-\cos x-\cos y-\cos z}$	$4\pi[18+12\sqrt{2}-10\sqrt{3}-7\sqrt{6}]$	15.672138	15.703623	15.676757
	$\times K^2[(2-\sqrt{3})(\sqrt{3}-\sqrt{2})]$ $=15.67249525$	(65812)	(9425)	(62456)
$I_{14}=\int_0^1\int_0^1\int_0^1\frac{\sin^{1/2}(xyz)}{[\lvert x+y-z\rvert]^{3/4}}\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$		0.29757191	0.297572564	fail
		(58444)	(7956)	
		0.365749083	0.365748588	
		(57733)	(7947)	
		0.30981519	0.309817251	
		(52901)	(7584)	
$I_{15}=\int_{-1}^1\int_{-1}^1\int_{-1}^1\lvert x^2+y^2+z^2-\frac{1}{4}\rvert\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$	$7+\frac{1}{120}\pi=7.026179936$	7.018352808	7.019202288	7.02053952
		(21143)	(9551)	(63167)

By comparison Romberg yields 15.641116 in 65^3 function evaluations [3] for I_{13} and 7.01853 in 65^3 function evaluations for I_{15}.

I_{14} with 20^3 functions evaluations, yields $\begin{cases}0.252831619\\0.300018810\\0.30973640\end{cases}$ by Gauss–Legendre.

I_{14} values are for I_{141}, I_{142} and I_{143}, respectively.

which is also the region of singular behaviour. Hence a special form for the integration range was introduced to avoid this problem.

Hence if $x'=\tanh\alpha_1$, and $y'=\tanh\beta_1$, with $\alpha_1=\alpha^3$ and $\beta_1=\beta^3$, then

$$x'=1-\frac{2}{\mathrm{e}^{2\alpha_1}+1}=-1+\frac{2}{1+\mathrm{e}^{-2\alpha_1}}\quad\text{and}\quad y'=1-\frac{2}{\mathrm{e}^{2\beta_1}+1}=-1+\frac{2}{1+\mathrm{e}^{-2\beta_1}},\tag{19}$$

where x' and y' satisfy the linear transformations

$$x=\tfrac{1}{2}(x'+1)\quad\text{and}\quad y=\tfrac{1}{2}(1-x)(y'+1).$$

Hence

$$1-x-y=\frac{1}{1+\mathrm{e}^{2\alpha_1}}\frac{1}{1+\mathrm{e}^{2\beta_1}},\tag{20}$$

so avoiding the cancellation.

The example I_4 causes some difficulties for the DE transformation because of the necessity to approach the singularity very closely—in fact well beyond the limit of overflow before the contributions to the integral have been made negligible by the sech^2 terms. This can be seen by considering the x-variable, say, which is at a distance from the singularity of order $\delta=$

$\exp^{-2}(\sinh\alpha)$ for large α. Hence the function values are of order $1/\delta^{3/4}$. On the other hand, the transformed function is multiplied by $\mathrm{sech}^2(\sinh\alpha)\cosh\alpha$ which for large α is of order $4\exp^{-2}(\sinh\alpha)\cosh\alpha$. Hence these terms are of the same order excluding the effect of $\cosh\alpha$, and relatively large α is required before the multiplying term dominates the singularity. The machine used for the computations has an exponent limit of 10^{38} and this was easily exceeded in this case. The effect is less marked for the simple $\tanh\alpha^n$ transformation which was able to handle this example.

The first column of values in Table 3 used $H = 0.1$ and the second column used $H = 0.2$ to give a comparison and test of achieved accuracy. To complete the comparison the DE rule results are shown in column 3. Even for the order of 10,000 points, values correct to 3 figures are obtained; this accuracy rises to around 7 figures at around 60,000 points. The DE rule is less good on these examples where the dimensionality effect of having to integrate a nonsingular function is present. By comparison the results from [3] which "ignore the singularity" are both expensive and inaccurate.

Finally, comparison was made with the results of Sugihara [7]. Sugihara combines the method of good lattice points with the DE rule for singular (and indeed general) integrands over a hypercube. Hence these examples are less general than those attempted in the earlier tables, in particular in Tables 2 and 3.

The number of quadrature points used by Sugihara for a given accuracy have been read off from the graphical results given in his paper. The comparison with the above methods is illustrated in Table 4. The integrals considered were

$$I_{16} = \int_0^1\int_0^1 \frac{\exp(-(x+y))}{\sqrt{xy}}\,\mathrm{d}x\,\mathrm{d}y = \pi\,\mathrm{erf}^2(1) = 2.2309851,$$

$$I_{17} = \int_0^1\int_0^1 \frac{\mathrm{d}x\,\mathrm{d}y}{(0.1+x+y)^2\sqrt{\sin\pi x + \sin\pi y}},$$

$$I_{18} = \int_0^1\int_0^1\int_0^1 \frac{\exp(-(x+y+z))}{\sqrt{xyz}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z = (\pi)^{3/2}\,\mathrm{erf}^3(1) = 3.3323071,$$

$$I_{19} = \int_0^1\int_0^1\int_0^1 \frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{(0.1+x+y+z)^2\sqrt{w(x)w(y)+w(y)w(z)+w(z)w(x)}},$$

where

$$w(\alpha) = \sin\pi\alpha.$$

In all four cases the accuracy obtained for a given number of points is comparable across the

Table 4

Integral	tanh rule, $n = 3$		Sugihara [7]
	Error	Number of points	Number of points
I_{16}	$-4.9(-6)$	355	200
I_{17}	$1.5(-7)$	1168	900
I_{18}	$-2.1(-7)$	13786	13000
I_{19}	$6.8(-5)$	10763	11000

methods. The integrals were also computed using the DE rule and again the two-dimensional cases gave similar accuracy; I_{16} reaching an error of 0.2(− 7) in 854 points (Sugihara used about 800 points), and I_{17} reaching 0.21(− 6) in 611 points (Sugihara using 500). However as in Table 3 the three-dimensional results were less good than either the $\tanh t^3$ transformation or than Sugihara.

5. Conclusions

A number of conclusions can be drawn from these tests. Firstly, the slight gain in using an error function transformation with say $n = 3$ would only be significantly advantageous if the integrands were themselves expensive to evaluate, when any saving becomes worthwhile. The relevant simplicity of tanh in a product rule certainly is attractive when complications such as variable limits and higher dimensions are tackled. For general use it is unreasonable to expect a user to contend with nonstandard functions when the gain is not considerable. This could be overcome by publishing a minimum rational approximation to the required functions over the relevant range.

The DE transformation is generally the most efficient rule for singular, low dimensional integrands but this rule is less good for dealing with integrands with singular derivatives and can enhance overflow problems in some cases. The rule is less good if singularities are absent and this can prove a problem in high dimensional quadratures where the singularity affects only one of the dimensions. The choice reduces to one of robustness with a slight loss of speed against efficiency with occasional failures. Equally a method which will cope with variable limit singularities will not be quite as fast as a more restricted algorithm for a specific integration range such as that of Sugihara.

The capability of the methods on the integrals with their singularities on internal curves shows efficiency and the experience gained in running the algorithm suggests a high level of robustness. On the three-dimensional cases it is of note that I_{14} is particularly hard with singular derivatives from the $\sin^{1/2}(xyz)$ term compounded with a power of $\frac{3}{4}$ in the denominator.

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