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The tanh transformation for double integrals with singularities—a progressive rule

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Abstract: Two transformation methods are extended to the numerical evaluation of two dimensional singular quadratures. These are both based on the tanh transformation and the resulting high order behaviour of the trapezoidal rule. Tests are carried out on some examples for which analytic results are also known.

Keywords: tanh transformation, singular two-dimensional quadrature, C.R. category 5.16.

1. Introduction

The use of transformations for the efficient evaluation of singular one-dimensional integrals has received some considerable attention recently. The principle involved is to try a transformation such as

$$x = g(t) \tag{1}$$

to a quadrature of the form

$$I = \int_{-1}^{1} f(x)\, dx \tag{2}$$

to yield an integral

$$I = \int f(g(t))g'(t)\, dt. \tag{3}$$

If $g'(t)$ has strong zeros in the region of the singularities of $g(x)$ (usually, and without loss of generality at the end points of the interval) then these singularities are removed from the new integrand $f(g(t))g'(t)$. A conventional quadrature rule may then be applied. In addition if it can be devised that the new integrand vanishes with all its derivatives at the end points, then it follows from the Euler–Maclaurin summation formula that the trapezoidal rule behaves as a very high order technique. One such successful transformation is to set

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

and this has been studied in one-dimension by Takahasi and Mori [1]; Mori [2]; Evans, Forbes and Hyslop [3] and Mori [4]. The higher derivatives of $g'(t)$ vanish exponentially at $\pm\infty$, the transformed end points, and the trapezoidal rule is therefore very effective.

Double integrals with singularites are also commonly encoutered and the question of whether these one-dimenional techniques can be extended to two-dimensions arises. It is the simplicity of the implementation of the tanh rule in [3] which encourages study of the two-dimensional case for this rule.

2. The formulation of the rule

The integral being considered is

$$I = \int_{a_2}^{b_2}\int_{a_1}^{b_1} F(x', y')\,\mathrm{d}x'\,\mathrm{d}y', \tag{4}$$

where singularities occur at the boundary of the region of integration. These may be singularities of the integrand itself or its derivatives. A linear transformation gives the form

$$I = \left(\frac{b_1 - a_1}{2}\right)\left(\frac{b_2 - a_2}{2}\right)\int_{-1}^{1}\int_{-1}^{1} F(x', y)\,\mathrm{d}x\,\mathrm{d}y, \tag{5}$$

where

$$x' = \frac{b_1 - a_1}{2}x + \frac{b_1 + a_1}{2}$$

and

$$y' = \frac{b_2 - a_2}{2}y + \frac{b_2 + a_2}{2}.$$

Hence setting

$$x = \tanh \alpha^n \quad \text{and} \quad y = \tanh \beta^n, \tag{6}$$

yields

$$I = n^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\tanh \alpha^n, \tanh \beta^n)(\alpha\beta)^{n-1}\operatorname{sech}^2 \alpha^n \operatorname{sech}^2 \beta^n\,\mathrm{d}\alpha\,\mathrm{d}\beta, \tag{7}$$

where

$$f(x, y) = \left(\frac{b_1 - a_1}{2}\right)\left(\frac{b_2 - a_2}{2}\right)F(x', y').$$

Two approaches were made to implementing a method based on equation (7). In the first, the infinite region was split into a set of concentric circles, the integrals round each circle being found by a Clenshaw–Curtis rule. The trapezoidal rule was then applied to these integrals with much philosophy of the one-dimensional approach. That is steps are taken away from the origin until two successive circle integrals give no significant contribution to the quadrature. This fixes the outer range of integration and then subdivision to convergence completes the process. Hence the substitution

$$\alpha = r\cos\theta \quad \text{and} \quad \beta = r\sin\theta, \tag{8}$$

is used to give

$$I = n^2 \int_0^{\infty} \int_0^{2\pi} G(r \cos \theta,\ r \sin \theta) r \, \mathrm{d}r \, \mathrm{d}\theta, \tag{9}$$

where

$$G(\alpha,\ \beta) = (\alpha\beta)^{n-1} \operatorname{sech}^2 \alpha^n \operatorname{sech}^2 \beta^n f(\tanh \alpha^n,\ \tanh \beta^n). \tag{10}$$

The trapezoidal rule then yields

$$I = n^2 h^2 \sum_{i=1}^{m} i \int_0^{2\pi} G(ih \cos \theta,\ ih \sin \theta) \, \mathrm{d}\theta, \tag{11}$$

where the initial steps with say length $h_0(=0.5$ possibly) determine the outer limit M so that after sub-division $hm = M$. The end points of the quadrature are hence ignored as the contribution at these points is negligible. Clenshaw–Curtis quadrature was employed in a progressive manner to evaluate the integrals from 0 to 2π, and $n = 3$ was found to be effective.

The alternative approach was to use the trapezoidal rule on both dimensions, now instigating a search in two variables and evaluating equation (7) in the form:

$$I = 4n^2 h_1 h_2 \sum_i \sum_j \left(f\left(\tanh \alpha_i^n,\ \tanh \beta_j^n\right)\left(\alpha_i \beta_j\right)^{n-1} \operatorname{sech}^2 \alpha_i^n \operatorname{sech}^2 \beta_j^n \right), \tag{12}$$

where α_i and β_j are the trapezoidal rule points and i and j cover the region defined below. The step lengths in the α and β directions are h_1 and h_2 and any integrand values on the boundary are ignored as these are negligible by the search procedure. Hence the internal weight is 4 throughout the region.

To make this method progressive, the search pattern requires some care.

The region is divided into four quadrants each of which is treated as follows. A routine is written which for a given β will search out along the α direction until two successive values of the integrand yield no significant contribution to the integral. This reduces the chances of a zero in the integrand prematurely terminating the search. The step size for this search is h_0 which is chosen to give a reasonable first approximation to the integral, without being too coarse that the upper limits are then poorly over estimated, resulting in extra unnecessary function evaluations especially at the next sub-division stage.

An internal search is made for values of β also in steps of h_0 from the origin. A set of upper limits is produced and eventually β becomes large enough that the search routine terminates at its starting point. In this way the upper limit of β is fixed. Each function evaluation is added into an accumulator as it is generated and the conclusion of the search phase yields a first approximation to the integral.

Two procedures are used for progressive sub-division to convergence. All the upper limits found in the first stage are stored. Along an existing β value the intermediate points can be simply evaluated and added into the accumulator. For the intermediate β values (shown by thin lines in the diagram) a search is required with the current step h (which will be some fraction of h_0 of the form $h_0/2^n$ at the nth step). Hence the progressive nature of the algorithm is obtained

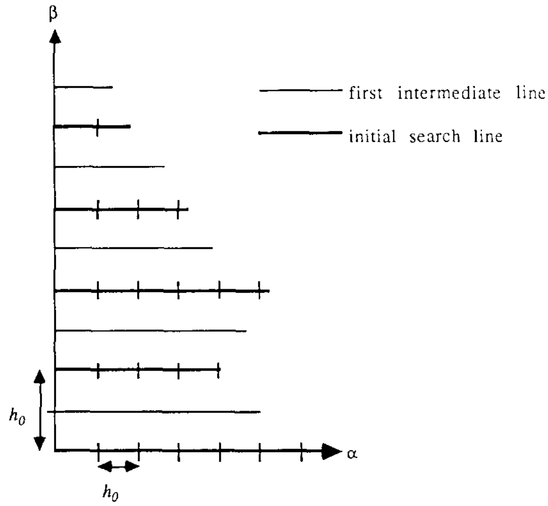

Fig. 1.

in that old function evaluations are re-used in the higher precision sweeps. This process is illustrated in Fig. 1.

3. The precision of the integrand

In one-dimension, to evaluate singular integrals methods require accurate function evaluations near to the singularity. This is traditionally overcome by providing two parameters for the function, one the normal value x and the other the distance from the singularity to x. Hence for example to evaluate $1.0/\sqrt{1-x^2}$ with x close to 1.0 cancellation will occur as soon as x has a decimal representation with figures common to 1.0. By writing $x = 1 - \epsilon$ and providing the parameter ϵ full accuracy can be maintained and the function $1.0/\sqrt{(1+x)\epsilon}$ is coded. With the tanh transformation (and indeed the more general transformation in Aihie and Evans [6]) the value of ϵ is known accurately as the singularity is moved to infinity so that $\tanh x = 1 - 2e^{-x}/(e^x + e^x) = 1 - \epsilon$ which yields the required value without cancellation. Just how serious this problem is depends on the arithmetic of the machine and the required accuracy. The number of significant figures of accuracy and the smallest representable number are the determining factors. In two dimensions the problem is less acute than in one as the singularities are of similar severity but the large numbers for the values of f near the singularities are now multiplied by *two* small ϵ values. Hence one requires to approach the singularity less closely for a given accuracy. Despite this a double parameter approach was found to be just necessary for the integrand $1.0/(1.0 - xy)$ which was re-coded as $1.0/(\epsilon + \delta - \epsilon\delta)$ where $x = 1 - \epsilon$ and $y = 1 - \delta$.

4. Results and conclusions

Table 1 shows a comparative performance of the new rules. The table contains the test integrals, the analytic values and the results obtained using Romberg and Gauss–Legendre

Table 1

Integrals	Analytic values	Romberg [a]	Gauss–Legendre [a]	Clenshaw–Curtis and trapezoidal rule [a]	tanh product rule [a]		
					$n=1$	$n=2$	$n=3$
$I_1=\int_0^1\int_0^1\frac{\mathrm{d}x\,\mathrm{d}y}{1-xy}$	$\pi^2/6$	−1.86 (4)	−1.17 (−4)	−1.41 (−5)	−7.30 (−7)	−4.56 (−7)	−2.09 (−6)
	1.644934	(2^{18})	(4096)	(3840)	(8213)	(3597)	(1975)
$I_2=\int_{-1}^1\int_{-1}^1\frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{1-x^2y^2}}$	$2\pi\ln 2$	−5.13 (−5)	−1.91 (−6)	−1.20 (−6)	−1.61 (−8)	−4.59 (−9)	9.41 (−5)
	4.3551722	(32060)	(4096)	(3840)	(8800)	(3653)	(1973)
$I_3=\int_{-1}^1\int_{-1}^1\frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{2-x-y}}$	$\frac{16}{3}(2-\sqrt{2})$	6.94 (−6)	−1.07 (−6)	3.10 (−7)	−1.16 (−6)	−1.54 (−7)	−4.80 (−8)
	3.1241943	(32060)	(4096)	(3840)	(7660)	(3535)	(1958)
$I_4=\int_{-1}^1\int_{-1}^1\frac{\mathrm{d}x\,\mathrm{d}y}{\sqrt{3-x-2y}}$	$\frac{4}{3}\sqrt{2}[3\sqrt{3}-2\sqrt{2}-1)$	9.73 (−5)	−1.40 (−6)	0.0	−1.05 (−6)	−2.91 (−7)	−1.98 (−7)
	2.5790076	(32060)	(4096)	(8153)	(7558)	(3514)	(1956)
$I_5=\int_0^1\int_0^1(xy)^{1/2}\,\mathrm{d}x\,\mathrm{d}y$		−1.44 (−2)	−1.35 (−2)	1.16 (−4)	−1.10 (−6)	−2.53 (−7)	−1.80 (−7)
	4.0	(32060)	(4096)	(6786)	(8864)	(4532)	(3542)
$I_6=\int_{-1}^1\int_{-1}^1\lvert x^2+y^2-0.25\rvert\,\mathrm{d}x\,\mathrm{d}y$	$\frac{5}{3}+\frac{1}{16}\pi$	−5.90 (−7)	−1.94 (−5)	4.83 (−8)	1.69 (−5)	8.24 (−6)	4.95 (−4)
	1.8630162	($2^{12}.3^2$)	(4096)	(2944)	(10057)	(4453)	(1961)
	8/15	−6.25 (−5)	−2.13 (−3)	7.31 (−8)	−1.80 (−3)	−4.82 (−3)	−9.49 (−3)
$I_7=\int_0^1\int_0^1\lvert x-y\rvert^{1/2}\,\mathrm{d}x\,\mathrm{d}y$	0.5333333	(2^{14})	(4097)	(7119)	(10057)	(3441)	(2751)

[a] The figures in brackets represent the number of function evaluations.

together with the results of the new rules. The test examples were chosen to allow comparison with Davis and Rabinowitz's results [5] and to have analytic values.

In general the new rules perform very well. However it is less easy to achieve a required accuracy by successive doubling of points as in one-dimension as the number of points used will grow impractically after one doubling. In the tanh product rule the underlying grid is fixed in the initial choice of h and a doubling in each dimension yields the results quoted. The tanh product rule is most efficient with the values of $n = 3$ and 5.

The doubling problem is less marked with the Clenshaw–Curtis and trapezoidal rule combination as each integral along a circle is accurately evaluated, and no more extra points are then needed if sub-division in the trapezoidal rule takes place. As in one-dimension, increasing n to 7 or above makes the integrand very steep sided and accuracy falls off.

Integrals I_6 and I_7 are different from the earlier examples having singular derivatives along a curve in the range of integration. As one might expect a trapezoidal product rule with no transformation performs quite well in that a 64 * 64 rule yields 1.864304 for I_6 and 0.532604 for I_7. The error depends on f'' rather than some higher more singular derivative. The Clenshaw-Curtis, trapezoidal rule combination gives very good accuracy for these examples as the tanh transformation enhances the effectiveness of the trapazoidal rule because it is operating on a set of Clenshaw quadratures which are well-known for coping with derivative singularities.

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