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Quadrature Formulas Obtained by Variable Transformation

Hidetosi Takahasi
Faculty of Science, University of Tokyo, Bunkyo-ku, Tokyo, Japan

Masatake Mori
Research Institute for Mathematical Sciences, Kyoto University, Kitasirakawa, Kyoto, Japan

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Abstract. Quadrature formulas suitable for evaluation of improper integrals such as $\int_{-1}^{1} f(x)(1-x)^{-\alpha}(1+x)^{-\beta}dx$, $\alpha, \beta < 1$ are obtained by means of variable transformations $x = \tanh u$ and $x = \operatorname{erf} u$, and subsequent use of trapezoidal quadrature rule. Error analysis is carried out by the method of contour integral, and the results are confirmed on several concrete examples. Similar formulas are also obtained to accelerate the convergence of infinite integrals $\int_{-\infty}^{\infty} f(x)\,dx$ by means of variable transformations $x = \sinh u$ and $x = \tan u$.

1. Introduction

Variable transformation is a well-known technique for evaluation of improper integrals. However, its success strongly depends on a proper choice of the mapping function, which seems to have been left to the ingenuity of each mathematician, who is supposed to get a special mapping function tailored for each specific integrand (e.g. [2]). In contrast with that, Schwartz [7] has given a seemingly general prescription for such a transformation which is very efficient when applied to a large class of improper integrals. In the present paper we will give several quadrature formulas obtained according to similar ideas as Schwartz's. That is, the mapping function is so chosen that the singular points of the integrand is moved to infinity, which converts the improper integral into a convergent infinite one, and the trapezoidal rule with an equal mesh size is applied to the converted integral.

One might think that such a transform would simply exchange one difficulty for another, but this is not the case. Reasonably smooth convergent infinite integrals are easier to evaluate than those with finite limits. The use of the trapezoidal rule with an equal mesh size over $(-\infty, \infty)$ gives an unusually high accuracy as has been first noted by Goodwin [3]. Indeed it can be shown to be more efficient than any other quadrature formulas over $(-\infty, \infty)$ having an infinite number of sampling points provided the integrand is analytic over $(-\infty, \infty)$ [8].

The present work overlaps much of the Schwartz's results [7][1]. Nevertheless we feel that a more detailed exposition of this technique, having in mind its use in the library routines, is fully justified. We will also give another transformation which converts an infinite integral into a finite integral of a periodic function.

We assume that the integrand of the given integral is analytic over the range of integration except at the end points, and apply the method of contour integral to error analysis [5, 6, 8, 9].

2. Generalities

Let

$$I = \int_a^b f(x)\,dx \tag{2.1}$$

be the integral to be evaluated. $f(x)$ is assumed to be analytic in a certain domain which includes the line segment (a, b). We make a change of variable by means of a substitution

$$x = \phi(u), \tag{2.2}$$

where $\phi(u)$ is analytic in a certain domain and maps the line segment $c \leqq u \leqq d$ onto $a \leqq x \leqq b$ monovalently. We then obtain the transformed integral

$$I = \int_c^d g(u)\,du \tag{2.3}$$

where

$$g(u) = f(\phi(u))\,\phi'(u). \tag{2.4}$$

It is also remarked that either or both of c and d may be infinite. The function $g(u)$ is also analytic in a certain domain including (c, d). Thus we can apply any known quadrature rule to (2.3), giving, say,

$$I_A = \sum_k A_k\, g(a_k). \tag{2.5}$$

Rewriting (2.5) in terms of the original function $f(x)$ we obtain a new quadrature formula

$$I_A = \sum_k A_k \phi'(a_k) f(\phi(a_k)) = \sum_k B_k f(b_k) \tag{2.6}$$

for the original integral (2.1), where $b_k = \phi(a_k)$ and $B_k = A_k \phi'(a_k)$ are the abscissas and the weights of this new formula.

The error for the formula (2.6)

$$\Delta I = \int_c^d g(u)\,du - \sum_k A_k\, g(a_k) \tag{2.7}$$

can be brought into a form of contour integral by the substitution of Cauchy's integral representation for $g(u)$ into (2.7), resulting in

$$\Delta I = \frac{1}{2\pi i} \oint_{\hat{C}} \hat{\Phi}(w)\, g(w)\, dw, \tag{2.8}$$

1 We are indebted to the referee for bringing this paper to our notice.

where

$$\hat{\Phi}(w) = \int_{c}^{d} \frac{du}{w-u} - \sum_{k} \frac{A_k}{w-a_k}. \tag{2.9}$$

The function $\hat{\Phi}(w)$, defined in the complex w-plane, will be called the *characteristic function* of the quadrature error [8, 9]. The path $\hat{C}$ is a contour enclosing the line segment (c, d) counterclockwise. The error estimation, i.e. the evaluation of the contour integral (2.8), can be carried out by the saddle point method [8].

The change of the variable w of integral (2.8) into z through the transformation

$$z = \phi(w) \tag{2.10}$$

yields another formula

$$\Delta I = \frac{1}{2\pi i} \oint_{C} \Phi(z) f(z)\, dz, \tag{2.11}$$

where the function $\Phi(z)$ is defined in the complex z-plane by

$$\Phi(z) = \Phi(\phi(w)) = \hat{\Phi}(w). \tag{2.12}$$

The formula (2.11) gives the quadrature error directly in terms of the original function $f(z)$. Hence $\Phi(z)$ is to be regarded as the characteristic function of the original formula (2.6). The path C is the mapped image of $\hat{C}$ from the w-plane into the z-plane by $z = \phi(w)$.

As we have shown in the papers [8, 9], it is very helpful for practical error estimation to have a contour map of the modulus of the characteristic function $|\Phi(z)|$ or $|\hat{\Phi}(w)|$ prepared for each quadrature formula. The choice between the two formulas (2.8) and (2.11) may be made according to convenience.

3. Quadrature Formulas for Improper Integrals

In this section we apply the variable transformation to the integration of an improper integral over the open interval $(-1, 1)$, i.e.

$$I = \int_{-1}^{1} f(x)\, dx, \tag{3.1}$$

where $f(x)$ may have singularities at one end or both ends of the interval.

(3.a) *The TANH-Rule.* If we take

$$x = \tanh u \tag{3.a.1}$$

as the mapping function, we have

$$I = \int_{-\infty}^{\infty} f(\tanh u) \frac{1}{\cosh^2 u}\, du. \tag{3.a.2}$$

Applying the trapezoidal rule we obtain the quadrature formula

$$I_A = h \sum_{n=-\infty}^{\infty} f(\tanh nh) \frac{1}{\cosh^2 nh}. \tag{3.a.3}$$

We will call (3.a.3) the TANH-rule.

The error of (3.a.3) is given as

$$\Delta I = I - I_A = \frac{1}{2\pi i} \int_{\hat{C}} \hat{\Phi}(w) f(\tanh w) \frac{1}{\cosh^2 w}\, dw, \tag{3.a.4}$$

where the characteristic function $\hat{\Phi}(w)$ is given by [8]

$$\hat{\Phi}(w) = \begin{cases} \dfrac{-2\pi i}{1-\exp(-2\pi i w/h)} \cong 2\pi i \exp(+2\pi i w/h); & \operatorname{Im} w > 0 \\ \dfrac{2\pi i}{1-\exp(+2\pi i w/h)} \cong -2\pi i \exp(-2\pi i w/h); & \operatorname{Im} w < 0. \end{cases} \tag{3.a.5}$$

The path $\hat{C}$ consists of two infinite lines running along both sides of the real axis. Hence we have the characteristic function $\Phi(z)$ in the z-plane

$$\Phi(z) = \hat{\Phi}(\operatorname{artanh} z) \cong \begin{cases} 2\pi i \left(\dfrac{1+z}{1-z}\right)^{+\pi i/h}; & \operatorname{Im} z > 0 \\ -2\pi i \left(\dfrac{1+z}{1-z}\right)^{-\pi i/h}; & \operatorname{Im} z < 0, \end{cases} \tag{3.a.6}$$

so that

$$\Delta I = \frac{1}{2\pi i} \int_C \Phi(z) f(z)\, dz, \tag{3.a.7}$$

where C is the mapped image of $\hat{C}$ in the z-plane.

It should be noted that the function artanh z is multi-valued so that each strip domain in the w-plane

$$W_m = \{w \mid -\pi/2 + m\pi < \operatorname{Im} w < \pi/2 + m\pi\}, \quad m = 0, \pm 1, \pm 2, \ldots \tag{3.a.8}$$

is mapped onto the whole z-plane cut along $(1, \infty)$ and $(-\infty, -1)$. Accordingly, the characteristic function (3.a.6) and hence the integrand of (3.a.7) should be defined on the Riemann surface so that the path C may also run outside the principal sheet.

The contour for $|\Phi(z)| = \varepsilon$ is the mapped image of the contour $|\hat{\Phi}(w)| = \varepsilon$ in the w-plane, which is approximately a pair of straight lines given by $\operatorname{Im} w = \pm (h/2\pi) \log(2\pi/\varepsilon)$, and hence the former is given by a pair of circular arcs

$$x^2 + (y \pm \cot 2c_0)^2 = \frac{1}{\sin^2 2c_0}; \quad z = x + iy, \quad c_0 = (h/2\pi) \log(2\pi/\varepsilon) \tag{3.a.9}$$

which meet at $z = \pm 1$. It will be seen that only those curves for which $\varepsilon < 2\pi \cdot \exp(-\pi^2/h)$ fall in the principal sheet of the Riemann surface, as is shown in Fig. 1 for the case $h = 0.5$.

It should also be noted that any quadrature formula obtained by a variable transformation is subject to an *inherent* error, which cannot be avoided irrespective of the integrand, i.e. even when integrating constant. Assume the given function $f(x)$ to have the form

$$f(x) = (1 - x^2)^{-\alpha} f_1(x), \quad \alpha < 1 \tag{3.a.10}$$

where $f_1(x)$ is regular in a certain domain including the interval $[-1, 1]$. We use (3.a.4) and deform the contour $\hat{C}$ so as to be able to use the saddle point

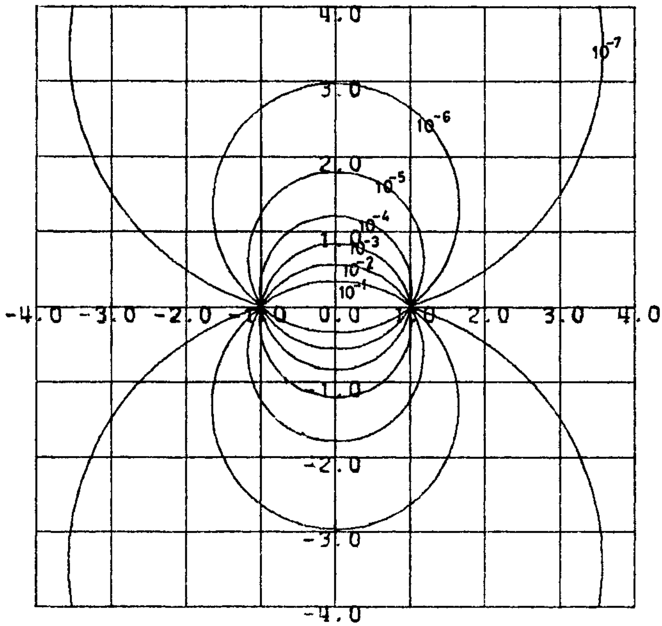

Fig. 1. The contour map of $|\Phi(z)|$ of the TANH-rule for $h=0.5$

method. Since the integrand

$$F(w) = \hat{\Phi}(w) \frac{1}{\cosh^2 w} (1-\tanh^2 w)^{-\alpha} f_1(\tanh w) \tag{3.a.11}$$

has singularities (poles or branch points) at $w = \pm \pi i/2$, we cannot move the path $\hat{C}$ beyond these points. Since the variation of (3.a.11) is dominated, when h is small, by the rapid decay of $|\hat{\Phi}(w)| \cong 2\pi \exp(-2\pi|\mathrm{Im}\,w|/h)$ for large $|\mathrm{Im}\,w|/h$, we have, by taking the path $\hat{C}$ close to these singularities, a rough estimate for the error:

$$\varepsilon(h) \cong |\hat{\Phi}(\pm \pi i/2)| \cong 2\pi \exp(-\pi^2/h). \tag{3.a.12}$$

If we estimate (3.a.4) more precisely by the saddle point method, we would see that the exact error is $2\pi \exp(-\pi^2/h)$ multiplied by a factor of order 1 which depends on α. This amount of error cannot be avoided whenever we use TANH-rule, i.e. even when $\alpha=0$, since the singularity is also contained in $\hat{\Phi}(w)/\cosh^2 w$. Larger error will be introduced if $f(z)$ has singularities outside the real axis.

Since (3.a.3) involves an infinite sum, an additional error ε_t due to the truncation, i.e. the replacement of $\sum_{n=-\infty}^{\infty}$ by $\sum_{n=-N/2}^{N/2}$, should be considered. For a given number of terms $N+1 \cong N$, ε_t increases when h is diminished, while $\varepsilon(h)$ is then diminished, and hence we expect a certain optimum value for h. If we use the form (3.a.10) for $f(x)$, ε_t is approximately given by

$$\varepsilon_t \cong \exp[-(1-\alpha)Nh]. \tag{3.a.13}$$

The minimum error is obtained for a given N when

$$\frac{d}{dh}\{\varepsilon(h)+\varepsilon_t\}=\frac{d}{dh}\{\exp(-\pi^2/h)+\exp(-(1-\alpha)Nh)\}=0$$

or

$$\exp(-\pi^2/h)\cong\exp[-(1-\alpha)Nh] \tag{3.a.14}$$

if we drop the factor of order 1 outside the exponential function. This yields the optimum value of h:

$$h=\frac{\pi}{\sqrt{(1-\alpha)N}}. \tag{3.a.15}$$

Substituting this into (3.a.12), we see that the dominating factor in the error can be written as

$$\varepsilon(N)\cong 2\pi\exp\left(-\pi\sqrt{1-\alpha}\,N^{\frac{1}{2}}\right) \tag{3.a.16}$$

in terms of number N of the sampling points. It must be noted that (3.a.16) has been derived with the assumption that $f_1(z)$ in (3.a.10) is everywhere regular except on the real axis. If it has any singularity elsewhere in the complex plane, a more detailed analysis would be needed, perhaps with the aid of Fig. 1 (or a similar figure for each specific value of h). In any case, however, we can expect an asymptotic form of $\varepsilon(N)$ which is more or less similar to (3.a.16) above.

(3.b) *The ERF-Rule.* If we take

$$x=\operatorname{erf}u=\frac{2}{\sqrt{\pi}}\int_0^u\exp(-t^2)\,dt \tag{3.b.1}$$

as the mapping function, we have

$$I=\int_{-\infty}^{\infty}f(\operatorname{erf}u)\frac{2}{\sqrt{\pi}}\exp(-u^2)\,du. \tag{3.b.2}$$

Applying the trapezoidal rule as in (3.a), we have

$$I_A=\frac{2}{\sqrt{\pi}}h\sum_{n=-\infty}^{\infty}f(\operatorname{erf}nh)\exp(-n^2h^2), \tag{3.b.3}$$

which will be called the ERF-rule.

If we assume the same form (3.a.10) for $f(x)$, the error can be estimated by studying the analytic behavior of the function

$$F(w)=\hat{\Phi}(w)\frac{2}{\sqrt{\pi}}\exp(-w^2)(1-\operatorname{erf}^2 w)^{-\alpha}. \tag{3.b.4}$$

If the functions $1\pm\operatorname{erf}w$ have any zeros which are finite, the path $\hat{C}$ of the integral (2.8) cannot be moved beyond these zeros. To locate these zeros we make use of the map of $\operatorname{erf}w$ in the first quadrant of the w-plane which is given in Fig. 2 showing the contours of its moduli and phases. The map for the other quadrants can be obtained by reflection with respect to the real and the imaginary axes, since $\operatorname{erf}w$ is a real odd analytic function. It will be seen from this figure that the function $\operatorname{erf}w$ has an infinite array of zeros lying closely along the line

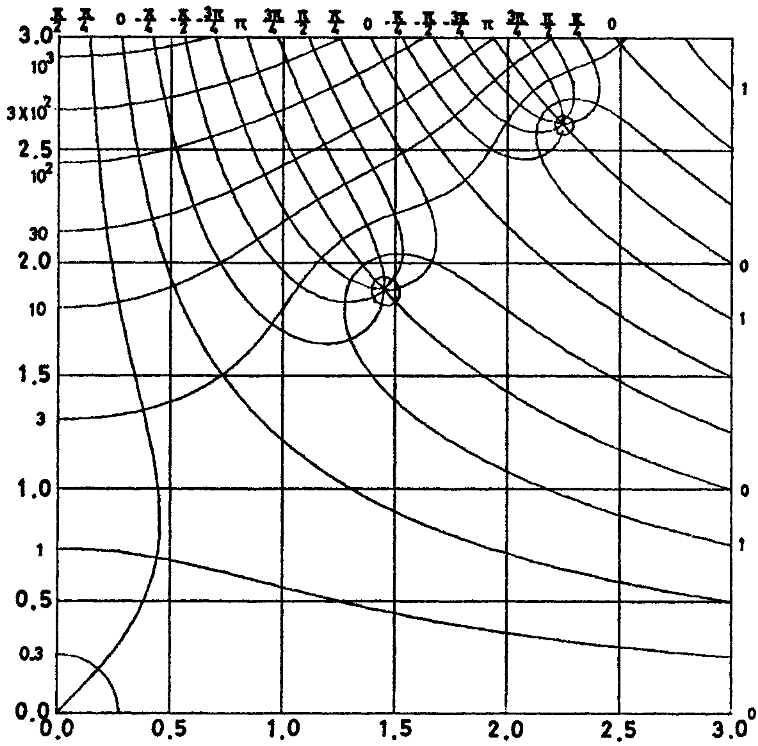

Fig. 2. The altitude map of modulus and phase of erf w

$v = u$ $(w = u + iv)$ and also that the zeros of $1 + \operatorname{erf} w$, i.e. the points satisfying $\operatorname{erf} w = -1$, are located in the close vicinity of these zeros. The position of the singular points that are located nearest to the origin and the real axis are given by $\pm w_0$ and $\pm \bar{w}_0$, where

$$w_0 \cong 1.35 + 1.99i. \tag{3.b.5}$$

Thus, by deforming the path $\hat{C}$ very close to these points, we have a rough estimate of the error of the present formula:

$$\varepsilon(h) \cong 2\pi |\hat{\Phi}(w_0)| \cong 2\pi \exp\left(-\frac{12.5}{h}\right). \tag{3.b.6}$$

Similar consideration as has been made for the foregoing example leads to an expression for the error for a given number of terms, given as

$$\varepsilon(N) \cong 2\pi \exp\left(-3.4 \sqrt[3]{1-\alpha}\, N^{2/3}\right). \tag{3.b.7}$$

Comparing (3.b.7) with (3.a.16), we see that the ERF-rule is in general superior to the TANH-rule for integrands such that $f_1(x)$ is regular in the whole z-plane.

When $\alpha = 0$, $F(w)$ has no singularity in the finite w-plane. Even in that case we have an error of the order of $\exp(-\pi^2/h^2)$ which is obtained by making the path $\hat{C}$ pass through $w = \pm \pi i/h$, the saddle points of $F(w)$. We may call this the inherent error of the present formula.

(3.c) *The IMT-Rule.*

Another formula, which is due to Iri, Moriguti and Takasawa [4], is obtained by the change of variable

$$x = \phi(u) = \frac{1}{Q} \int_{-1}^{u} \exp\left(-\frac{2}{1+t} - \frac{2}{1-t}\right) dt, \tag{3.c.1}$$

$$Q = \int_{-1}^{1} \exp\left(-\frac{2}{1+t} - \frac{2}{1-t}\right) dt \tag{3.c.2}$$

which maps the interval $(-1, 1)$ onto itself. Since all the derivatives of $\phi(u)$ vanish at -1 and $+1$ we can again apply the trapezoidal rule with an equal mesh size of $h = 1/N$ to the transformed integral. We call this the IMT-rule. It is also applicable to improper integrals. It can be shown [4] that, if the integrand is of the same form as (3.a.10), the dominating factor of the inherent error is

$$\varepsilon(N) \cong 2\pi \exp\left(-\sqrt{4\pi(1-\alpha)}\, N^{\frac{1}{2}}\right). \tag{3.c.3}$$

Hence the IMT-rule is about as efficient as the TANH-rule when $f(x)$ is regular except at $z = \pm 1$.

4. Numerical Examples for TANH-, ERF- and IMT-Rule

The above three rules are applied and compared for the following two samples of improper integrals.

(4.i)
$$\int_{-1}^{1} \frac{dx}{(x-2)(1-x)^{\frac{1}{4}}(1+x)^{\frac{3}{4}}} = -1.9490\ldots$$

(4.ii)
$$\int_{-1}^{1} \frac{\cos \pi x}{(1-x)^{\frac{1}{2}}}\, dx = -0.69049\ldots.$$

Figs. 3 and 4 show the errors in the results of application of the above quadrature rules to these examples as a function the number N of the sampling points actually used. These curves have been obtained by an optimal choice of the truncation points, i.e. by that of the value N for each value of h. This optimization, while necessary in order to obtain a smooth curve, is not essential for the practical application of these formulas.

It will be evident from these figures that the ERF-rule is far superior to the TANH-rule and the IMT-rule for the same number of the sampling points. We have already seen this in the error analysis. A merit of the TANH-rule may be found, however, in the simplicity of generating the sampling points and the weights in the process of integration.

In (4.i) the error due to the poles of the integrand at $x = 2$ becomes dominant in comparison with that due to the singularities at the ends of the interval, except in the case of TANH-rule, in which case both errors are of nearly the same order of magnitude, because the part of the real axis $y = 0$, $|x| > 1$ is mapped onto the line $\operatorname{Im} w = \pi/2 + m\pi$ on which $|\hat{\Phi}(w)|$ takes the constant value $\cong 2\pi \exp(-\pi^2/h)$.

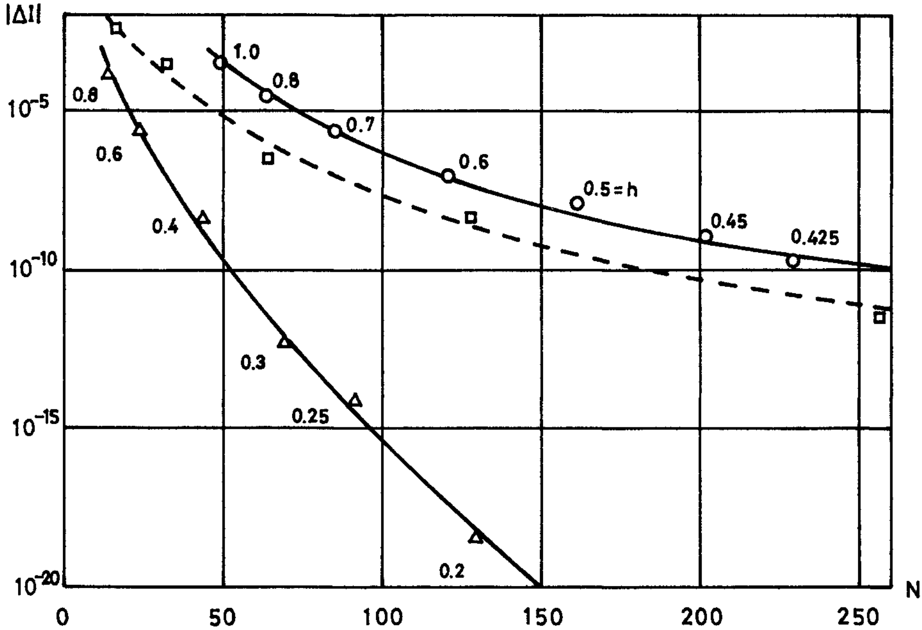

Fig. 3. The computed error of $\int_{-1}^{1} 1/\{(x-2)(1-x)^{\frac{1}{4}}(1+x)^{\frac{3}{4}}\}\,dx$

(—○— TANH-rule, —▲— ERF-rule, --□-- IMT-rule)

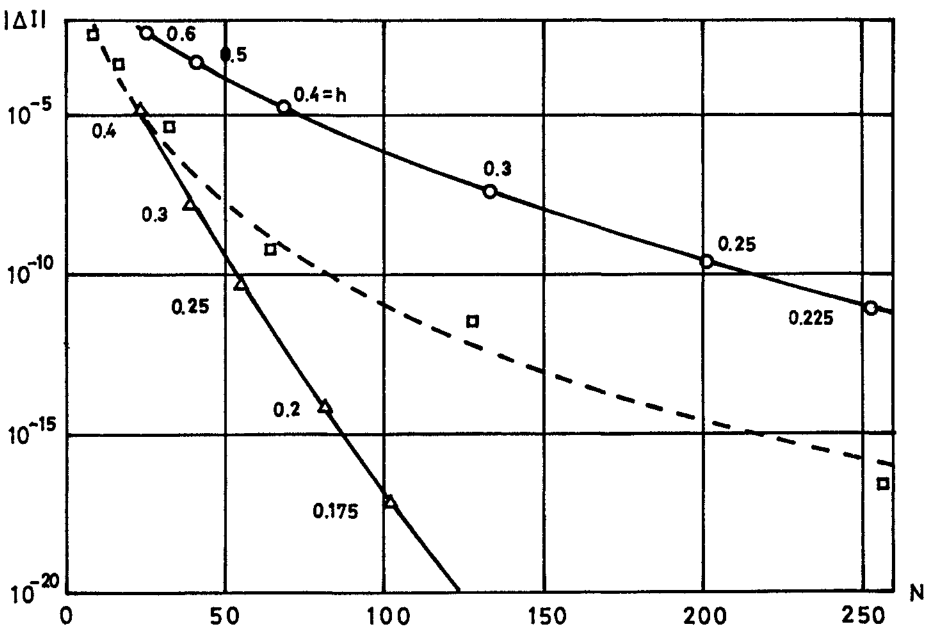

Fig. 4. The computed error of $\int_{-1}^{1} (\cos \pi x)/\sqrt{1-x}\,dx$

(—○— TANH-rule, —▵— ERF-rule, --□-- IMT-rule)

In the example (4.ii), the main contribution to the error comes from the saddle points, the existence of which is due to the fast growth of $|\cos \pi w|$ and the rapid decay of $|\hat{\Phi}(w)|$ in both directions along the imaginary axis.

It should be remarked that special caution is required in the evaluation of the integrand to avoid the loss of significant figures due to cancellation as x tends to ± 1. One should make a direct substitution of $t = 1 - x = 1 - \tanh u = 2\exp(-2u)/(1 + \exp(-2u))$ or $t = 1 - x = 1 - \operatorname{erf} u = \operatorname{erfc} u$ into $1 - x$, if possible. In using computers one should also be aware of possible underflow troubles.

5. Quadrature Formulas for Slowly Convergent Integrals

Another example of the use of variable transformation is to accelerate the convergence of an infinite integral

$$I = \int_{-\infty}^{\infty} f(x)\, dx \tag{5.1}$$

whose integrands decay rather slowly as x goes to infinity. Such is the case when integrating $\int_{-\infty}^{\infty} (1 + x^2)^{-\frac{5}{4}} dx$, for example.

(5.a) *The SINH-Rule.* We put

$$x = \sinh u \tag{5.a.1}$$

in (5.1), so that we have

$$I = \int_{-\infty}^{\infty} f(\sinh u) \cosh u\, du. \tag{5.a.2}$$

If we apply the trapezoidal rule with a mesh size of h, we have a quadrature formula

$$I_A = h \sum_{n=-\infty}^{\infty} f(\sin nh) \cosh nh, \tag{5.a.3}$$

which will be called the SINH-rule. We have for the error

$$\Delta I = \frac{1}{2\pi i} \int_{\hat{C}} \hat{\Phi}(w) f(\sinh w) \cosh w\, dw, \tag{5.a.4}$$

where $\hat{\Phi}(w)$ is given by (3.a.5).

The approximate characteristic function $\Phi(z)$ expressed in the z-plane is written as

$$\Phi(z) = \hat{\Phi}(\operatorname{arsinh} z) \cong \begin{cases} 2\pi i \left(z + \sqrt{z^2 + 1}\right)^{+\frac{2\pi i}{h}}; & \operatorname{Im} z > 0 \\ -2\pi i \left(z + \sqrt{z^2 + 1}\right)^{-\frac{2\pi i}{h}}; & \operatorname{Im} z < 0. \end{cases} \tag{5.a.5}$$

The contour map of $|\Phi(z)|$ is obtained by the mapping of the straight lines $\operatorname{Im} w = \pm c_0$, $c_0 = (h/2\pi) \log(2\pi/\varepsilon)$ into the z-plane, and is given by a family of confocal hyperbolas

$$-\frac{x^2}{\cos^2 c_0} + \frac{y^2}{\sin^2 c_0} = 1 \tag{5.a.6}$$

with foci at $z = \pm i$.

By the transformation $z = \sinh w$, each strip domain W_m defined by (3.a.8) is mapped onto the whole z-plane cut along $(i, i\infty)$ and $(-i, -i\infty)$. In the principal sheet of the Riemann surface, $|\Phi(z)|$ takes its minimum value $\cong 2\pi \exp(-\pi^2/h)$ along the cuts $(i, i\infty)$ and $(-i, -i\infty)$, and $|\Phi(z)|$ can never become smaller than that minimum value over the whole principal sheet. Now, any non-trivial integrand $f(z)$ must have at least one singularity over the whole z-plane, either at a finite z or at infinity, and if it is at infinity, it must be an essential singular point since $f(z) \to 0$ as $z \to \pm\infty$. Let us first assume that there is a singular point at a finite z. Then we cannot move the path C beyond this point, so that an error in excess of the minimum value $2\pi \exp(-\pi^2/h)$ is to be expected. If, on the other hand, $f(z)$ has an essential singular point at $z = \infty$, $|f(z)|$ must become large towards some direction with $\arg z \neq 0, \pi$, and hence the path C cannot be moved to infinity either. In any case, an error of the order of

$$\varepsilon(h) \cong 2\pi \exp(-\pi^2/h) \tag{5.a.7}$$

cannot be avoided, the *best* case being given by an integrand having all its singularities on the cuts $(i, i\infty)$ and $(-i, -i\infty)$.

(5.b) *The TAN-Rule.* When the integrand $f(x)$ in (5.1) happens to be regular at $x = \infty$, the transformation

$$x = \tan u \tag{5.b.1}$$

turns out to give an exceedingly efficient quadrature algorithm. By this transformation, (5.1) is converted to a finite integral

$$I = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} f(\tan u) \frac{1}{\cos^2 u} du \tag{5.b.2}$$

of an analytic function $f(\tan u)/\cos^2 u$ which is periodic with period π and regular along the real axis including the end points $u = \pm\pi/2$ provided that the original integral is convergent. Since the trapezoidal rule with equally spaced sampling points is applicable for integration of periodic function over the whole period we have

$$I_A = h \sum_{n=-\frac{N}{2}}^{\frac{N}{2}-1} f(\tan nh) \frac{1}{\cos^2 nh} \quad (N\text{: even}), \tag{5.b.3}$$

in which $h = \pi/N$. We will call this formula the TAN-rule. The characteristic function $\hat{\Phi}(w)$ for (5.b.3) is again given by (3.a.5) [1], so that the error is given by the integral

$$\Delta I = \frac{1}{2\pi i} \int_{\hat{C}} \hat{\Phi}(w) f(\tan w) \frac{1}{\cos^2 w} dw, \tag{5.b.4}$$

and the path $\hat{C}$ is taken as a rectangle with a width equal to π, the period of $\tan w$.

The characteristic function $\Phi(z)$ for (5.b.3) expressed in the z-plane is given from (3.a.5) as

$$\Phi(z)=\begin{cases}\dfrac{-2\pi i}{1-\left(\dfrac{i-z}{i+z}\right)^{-N}}; & \operatorname{Im} z>0\\[2ex] \dfrac{2\pi i}{1-\left(\dfrac{i-z}{i+z}\right)^{+N}}; & \operatorname{Im} z<0.\end{cases} \tag{5.b.5}$$

Unlike (5.a.5) it is regular over each half-plane. The path C of integration should be two closed curves, each lying in the upper or lower half-plane and enclosing all the singularities in respective half-plane (Fig. 5). Such C exists even when $\Phi(z)$ is many-valued since $f(z)$ is regular at infinity.

The transformation $z=\tan w$ maps the straight lines $|\hat{\Phi}(w)|\cong\varepsilon$ in the w-plane into a family of circles

$$x^2+(y-\coth 2c_0)^2=\frac{1}{\sinh^2 2c_0}, \qquad c_0=(h/2\pi)\log(2\pi/\varepsilon) \tag{5.b.6}$$

in the z-plane. From this fact we can show that the error becomes smaller as all the singularities of the integrand get closer to $\pm i$.

It must be stressed that the present rule is only applicable to functions which are regular at infinity. If it is applied to a function having any singularity (e.g. branch point) at infinity, the approximation will be very poor.

Let us assume that the integrand $f(x)$ approaches 0 at $x\to\infty$ in such a way that

$$\lim_{x\to\infty} f(x)\,x^{\alpha}=\text{constant}, \qquad \alpha=\text{integer}\geqq 2. \tag{5.b.7}$$

The integrand in (5.b.2) vanishes at the end points $u=\pm\pi/2$ whenever α is greater than 2. When $\alpha=2$, it remains finite there, however, and we must compute it as the limit values $\lim_{x\to\infty} f(x)\,x^2$. This would give rise to a rather serious problem if the function $g(u)$ is to be computed by computer. In such cases, the

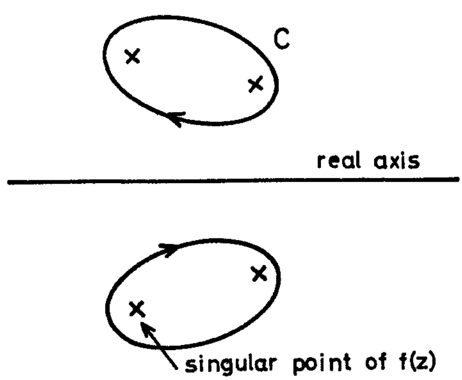

Fig. 5. The path C of the TAN-rule in the z-plane

use of the mid-point rule

$$I_A = h \sum_{n=-\frac{N}{2}}^{\frac{N}{2}-1} f\left(\tan\frac{\pi}{N}\left(\frac{1}{2}+n\right)\right)\frac{1}{\cos^2\frac{\pi}{N}\left(\frac{1}{2}+n\right)} \quad (N\text{: even}) \qquad (5.\text{b}.8)$$

will be recommended since it does not require the function values at the end of the interval. A possible drawback of the mid-point rule would arise when one employs an automatic procedure in which the step size is halved repeatedly until the required accuracy is attained. In that case all function values have to be computed anew in each step and one cannot make use of the values computed at preceeding steps.

6. Numerical Examples for SINH- and TAN-Rule

We apply the SINH- and the TAN-rule to the following integrals.

(6.i) $$\int_{-\infty}^{\infty} \frac{dx}{1+x^4} = 2.2214\ldots$$

(6.ii) $$\int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^{\frac{5}{4}}} = 2.3962\ldots.$$

In Fig. 6 the computed errors are shown as a function of the number N of the sampling points.

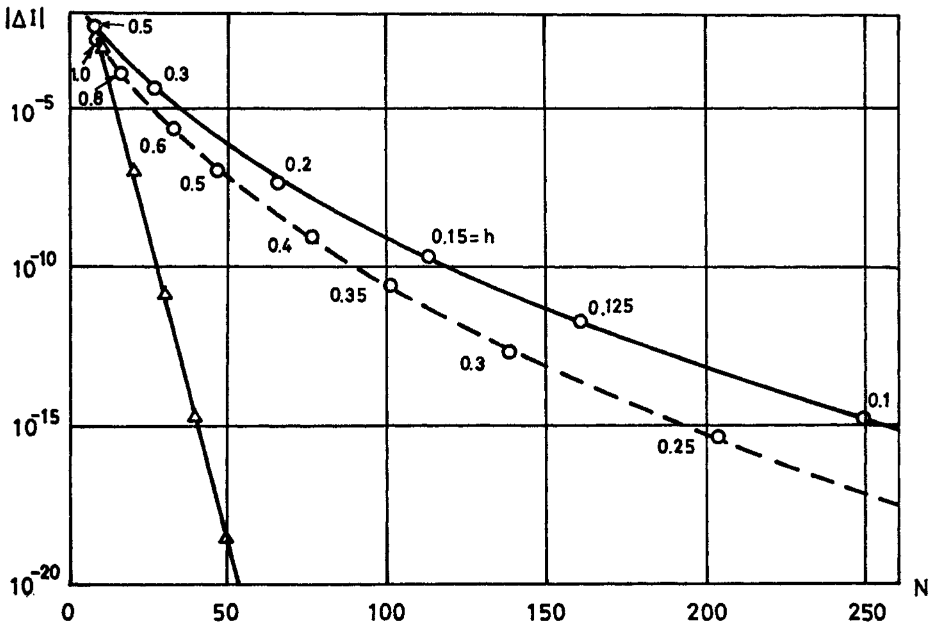

Fig. 6. The computed error of $\int_{-\infty}^{\infty}(1+x^4)^{-1}dx$
(—○— SINH-rule, —△— TAN-rule), and $\int_{-\infty}^{\infty}(1+x^2)^{-\frac{5}{4}}dx$ (--○-- SIN-rule)

The TAN-rule is obviously much more efficient than the SINH-rule for the integration of $1/(1+x^4)$ which is regular at infinity. The SINH-rule, on the other hand, can be applied to any function regardless of its analytic behavior as $x \to \pm\infty$, provided it is regular for finite real value of x. The error observed in (6.ii) with the SINH-rule is the error $\varepsilon(h)$ of (5.a.7). In (6.i), on the other hand, the error due to the poles of $1/(1+x^4)$ dominates over $\varepsilon(h) \cong 2\pi \exp(-\pi^2/h)$.

It would be a subordinate advantage of the SINH-rule that the position of the sampling point and the weight can be easily generated in the process of integration.

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M. Mori
Res. Institute for Mathematical Sciences
Kyoto University
Kitasirakawa, Kyoto
Japan