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IMT-type Quadrature Formulas Free from Intrinsic Errors

定数関数に対し正確な値を与えるＩＭＴ型数値積分公式

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Abstract　Let $x=\psi(t)$ ($\psi(0)=0$, $\psi(t)+\psi(1-t)=1$) be an IMT-type transformation for the numerical integration of $\int_0^1 f(x)dx$. This note points out that the transformation $x=\tilde{\psi}(t)$, where $\tilde{\psi}(t) = \int_0^{2t}\psi(s)ds$ ($0\leqq t\leqq 1/2$) and $\tilde{\psi}(t)+\tilde{\psi}(1-t)=1$, leads to a quadrature formula which is free from the intrinsic error (i.e., exact for $f(x)=1$) and as efficient as the original quadrature formula based on $x=\psi(t)$.

1. Introduction

We consider the numerical integration of

$$I = \int_0^1 f(x)dx. \tag{1.1}$$

A numerical quadrature formula based on the change of variable $x=\psi(t)$ ($\psi(a)=0$, $\psi(b)=1$, $\psi'(a)=\psi'(b)=0$) is obtained by applying the trapezoidal rule to the transformed integral

$$I = \int_a^b f(\psi(t))\psi'(t)dt. \tag{1.2}$$

Among such formulas, the IMT formula [Iri-Moriguti-Takasawa 1970] and the DE (Double Exponential) formula [Takahasi-Mori 1974] are well known (cf. [Davis-Rabinowitz 1984], [Mori 1985]). The former employs

$$\psi_{IMT}(t) = (1/Q) \int_0^t \exp[-1/s-1/(1-s)]ds, \qquad Q = \int_0^1 \exp[-1/s-1/(1-s)]ds \tag{1.3}$$

as the function $\psi(t)$ to map the interval (0,1) onto itself (i.e., a=0, b=1 in (1.2)), and the latter adopts

$$\psi_{DE}(t) = (1/2)\tanh[(\pi/2)\sinh t] + 1/2, \tag{1.4}$$

which maps $(a,b)=(-\infty,\infty)$ onto (0,1).

The resulting quadrature formula in the case of (a,b)=(0,1) is then given by

$$S_N = h \sum_{i=1}^{N-1} f(\psi(ih))\psi'(ih), \tag{1.5}$$

where h=1/N. In the case of $(a,b)=(-\infty,\infty)$, on the other hand, the trapezoidal approximation to (1.2) (with mesh size h)

$$S = h \sum_{i=-\infty}^{\infty} f(\psi(ih))\psi'(ih) \tag{1.6}$$

involves infinitely many points (abscissas), which should be truncated to a finite number, say N, without deteriorating the degree of approximation; S_N will denote a sum of the form (1.6) with N terms.

We will define

$$E_N = E_N(f) = S_N - I, \tag{1.7}$$

which is the integration error for an integrand f(x). It is known that the IMT formula and the DE formula have the property:

> E_N decreases faster than any polynomial in 1/N as $N\to\infty$ for a class of integrands of practical interest that may possess integrable algebraic/logarithmic singularities at endpoints of interval of integration. (1.8)

One of the peculiar properties of such a quadrature formula is that it fails to integrate a constant function exactly, that is,

$$E_N(1) \neq 0. \tag{1.9}$$

The error $E_N(1)$ is called the intrinsic error of the formula, which we are particularly concerned with here. Both the IMT formula and the DE formula, as well as their variants [Mori 1978], [Murota-Iri 1982], do have the property (1.9). In fact, all the formulas based on the technique of change of variable found in the literature (cf., e.g., [Takahasi-Mori 1973], [Mori 1985]) have this property, too.

Very recently, however, it was pointed out by Prof. Iri (reported in [Nishii-Murota-Iri 1985]) that there exists such a transformation function $\psi(t)=\psi_U(t)$ that yields a quadrature formula which has the property (1.8) and is free from intrinsic errors, i.e.,

$$E_N(1) = 0 \quad \text{for } N \text{ even.} \tag{1.10}$$

The function $\psi_U(t)$ is the cumulative distribution function of the random variable

$$\sum_{j=1}^{\infty} U_j/2^j \tag{1.11}$$

where U_j $(j=1,2,...)$ are independent random variables each being subject to the uniform distribution over the unit interval (0,1). It can be shown [Iri-Kabaya 1985] that $\psi_U(t)$ satisfies the functional equation

$$\psi_U(t) = \int_0^{2t} \psi_U(s)ds \quad (0 \leq t \leq 1/2), \tag{1.12}$$

$$\psi_U(t) + \psi_U(1-t)=1.$$

See [Iri-Kabaya 1985] for other properties of $\psi_U(t)$.

Unfortunately, the quadrature formula using $\psi_U(t)$ turned out [Nishii-Murota-Iri 1985] to be far less efficient for general integrands $f(x)$ than the IMT-type formulas, as compared in Table 1.1. This note gives quadrature formulas with no intrinsic errors that are roughly as efficient as the known IMT-type formulas.

Table 1.1. Efficiency and Intrinsic Errors

(a,b)	Formula	Efficiency (Error $E_N(f)$)	Intrinsic Error $E_N(1)$
finite	$\psi_U(t)$	$\exp[-c(\log N)^2]$	0
(0,1)	IMT: $\psi_{IMT}(t)$	$\exp[-c\sqrt{N}]$	same as $E_N(f)$
	IMT-type DE*	$\exp[-cN/(\log N)^2]$	same as $E_N(f)$
	IMT-double**	$\exp[-cN/(\log N)^2]$	same as $E_N(f)$
	IMT-triple**	$\exp[-cN/(\log N\ (\log\log N)^2)]$	same as $E_N(f)$
infinite $(-\infty,\infty)$	DE: $\psi_{DE}(t)$	$\exp[-cN/(\log N)]$	same as $E_N(f)$

* [Mori 1978]; ** [Murota-Iri 1982]

2. Intrinsic-Error Free Formulas

In the following, we assume

$\psi(0)=0,\ \psi(1)=1\quad(\psi(t)=0 \text{ for } t<0,\ \psi(t)=1 \text{ for } t>1),$

$$\psi(t) + \psi(1-t) = 1, \tag{2.1}$$

$\psi'(0)=\psi'(1)=0$ ($\psi(t)$ is differentiable as many times as needed).

The Fourier transform of $\psi'(t)$ is defined by

$$\omega(\kappa) = \int_0^1 \psi'(t)\exp(i2\pi\kappa t)dt, \quad \kappa\in R. \tag{2.2}$$

The error $E_N(f)$ is expressed (see, e.g., [Murota-Iri 1982]) in terms of the Fourier coefficients $C_k=C_k(f)$ of the integrand of (1.2):

$$E_N(f) = 2\sum_{p=1}^{\infty} \operatorname{Re} C_{pN}(f), \tag{2.3}$$

$$C_k(f) = \int_0^1 f(\psi(t))\psi'(t)\exp(i2\pi kt)dt, \quad k\in Z. \tag{2.4}$$

The intrinsic error is then given by

$$E_N(1) = 2 \sum_{p=1}^{\infty} \omega(pN). \tag{2.5}$$

This expression indicates that if

$$\omega(2k) = 0 \quad (k=1,2,\ldots), \tag{2.6}$$

then the formula with $x=\psi(t)$ has no intrinsic errors for N even.

It is a rule of thumb that the efficiency for a general integrand $f(x)$ is measured by how fast $|\omega(\kappa)|$ decays as $|\kappa|\to\infty$. In fact, this is the case with the IMT-type formulas. We discuss this issue in Appendix.

Now our problem of designing an efficient intrinsic-error free quadrature formula is reduced to that of finding such a Fourier transform $\omega(\kappa)$ of a nonnegative function $\psi'(t)$ (or, a characteristic function of a symmetric probability distribution) that satisfies (2.6) and decreases as rapidly as possible as $|\kappa|\to\infty$.

Here we take notice of the following facts:

(1) The Fourier transform of $\psi'_U(t)$ (or, the characteristic function of (1.11)) is given by

$$\omega_U(\kappa) = \exp(i\pi\kappa) \prod_{j=1}^{\infty} \sin(\pi\kappa/2^j)/(\pi\kappa/2^j), \tag{2.7}$$

which satisfies (2.6) on account of the factor $\sin(\pi\kappa/2)/(\pi\kappa/2)$. That is, the factor corresponding to $U_1/2$ in (1.11) renders the quadrature formula using $\psi_U(t)$ free from intrinsic errors.

(2) The Fourier transform $\omega(\kappa)$ of the derivative of an IMT-type transformation function $\psi(t)$ tends to zero rapidly as $|\kappa|\to\infty$; e.g., for (1.3), it is known [Iri-Moriguti-Takasawa 1970] that

$$\omega_{IMT}(\kappa) = O(\exp[-c\sqrt{|\kappa|}]). \tag{2.8}$$

(3) The product of two characteristic functions is again a characteristic function of a probability distribution.

When given an efficient quadrature formula based on a transformation $x=\psi(t)$, we can construct an intrinsic-error free formula using the transformation $x=\tilde{\psi}(t)$ defined as follows. Let $\omega(\kappa)$ and $\tilde{\omega}(\kappa)$ be the Fourier transforms of $\psi'(t)$ and $\tilde{\psi}'(t)$, respectively. We define

$$\tilde{\omega}(\kappa) = \omega(\kappa/2)\ \exp(i\pi\kappa/2)\ \sin(\pi\kappa/2)\ /\ (\pi\kappa/2) \tag{2.9}$$

and $\tilde{\psi}'(t)$ to be the inverse Fourier transform of $\tilde{\omega}(\kappa)$. In terms of $\psi(t)$ and $\tilde{\psi}(t)$, this amounts to

$$\tilde{\psi}(t) = \int_0^{2t}\psi(s)ds \quad (0 \leqq t \leqq 1/2), \tag{2.10}$$

and

$$\tilde{\psi}(t) + \tilde{\psi}(1-t) = 1. \tag{2.11}$$

Then it is easy to see, based on the above-mentioned facts, that $x=\tilde{\psi}(t)$ is qualified as the transformation function satisfying (2.1), and that the resulting quadrature formula is free from intrinsic errors and roughly as efficient as the original formula with $x=\psi(t)$. To be more precise, the new formula will require at most twice as many function evaluations as the original one, since we have

$$|\tilde{\omega}(\kappa)| \leqq |(2/\pi\kappa)\ \omega(\kappa/2)|, \quad \kappa\neq 0, \tag{2.12}$$

from (2.9). Namely, we may expect the relation

$$|\tilde{E}_N(f)| \leqq |E_{N/2}(f)| \tag{2.13}$$

between the integration error $\tilde{E}_N$ of the new formula and that of the original one.

When $\psi(t)$ is a polynomial, the explicit form of $\tilde{\psi}(t)$ can be given; for example, when

$$\psi'(t) = ((2m+1)!/(m!)^2)\ t^m(1-t)^m, \quad m=2,3,$$

we have

$$\tilde{\psi}(t) = 8t^4(5-12t+8t^2) \quad (0\leq t\leq 1/2) \quad \text{for } m=2,$$

and

$$\tilde{\psi}(t) = 32t^5(7-28t+40t^2-20t^3) \quad (0\leq t\leq 1/2) \quad \text{for } m=3.$$

It may worth while noting that (1.12) shows that $\psi_U(t)$ is a fixed point of the transformation (2.10), i.e.,

$$\tilde{\psi}_U(t) = \psi_U(t).$$

3. Numerical Examples

We compare the quadrature formulas with $x=\psi(t)$ and $x=\tilde{\psi}(t)$ (cf. (2.10)) for the two choices $\psi(t) = \psi_{TANH}(t)$ and $\psi(t) = \psi_{IMTDE}(t)$, where

$$\psi_{TANH}(t) = (1/2)\tanh[(1/4)(1/(1-t)-1/t)] + 1/2, \tag{3.1}$$

$$\psi_{IMTDE}(t) = (1/2)\tanh[(\pi/2)\sinh[(\pi/4)(1/(1-t)-1/t)]] + 1/2. \tag{3.2}$$

The formula with $x=\psi_{IMTDE}(t)$ is the IMT-type double exponential formula of [Mori 1978]. The formula with $x=\psi_U(t)$ [Nishii-Murota-Iri 1985] is also considered.

The integration errors are observed for the following six integrand functions:

$$f_1(x) = 1, \qquad I = 1,$$

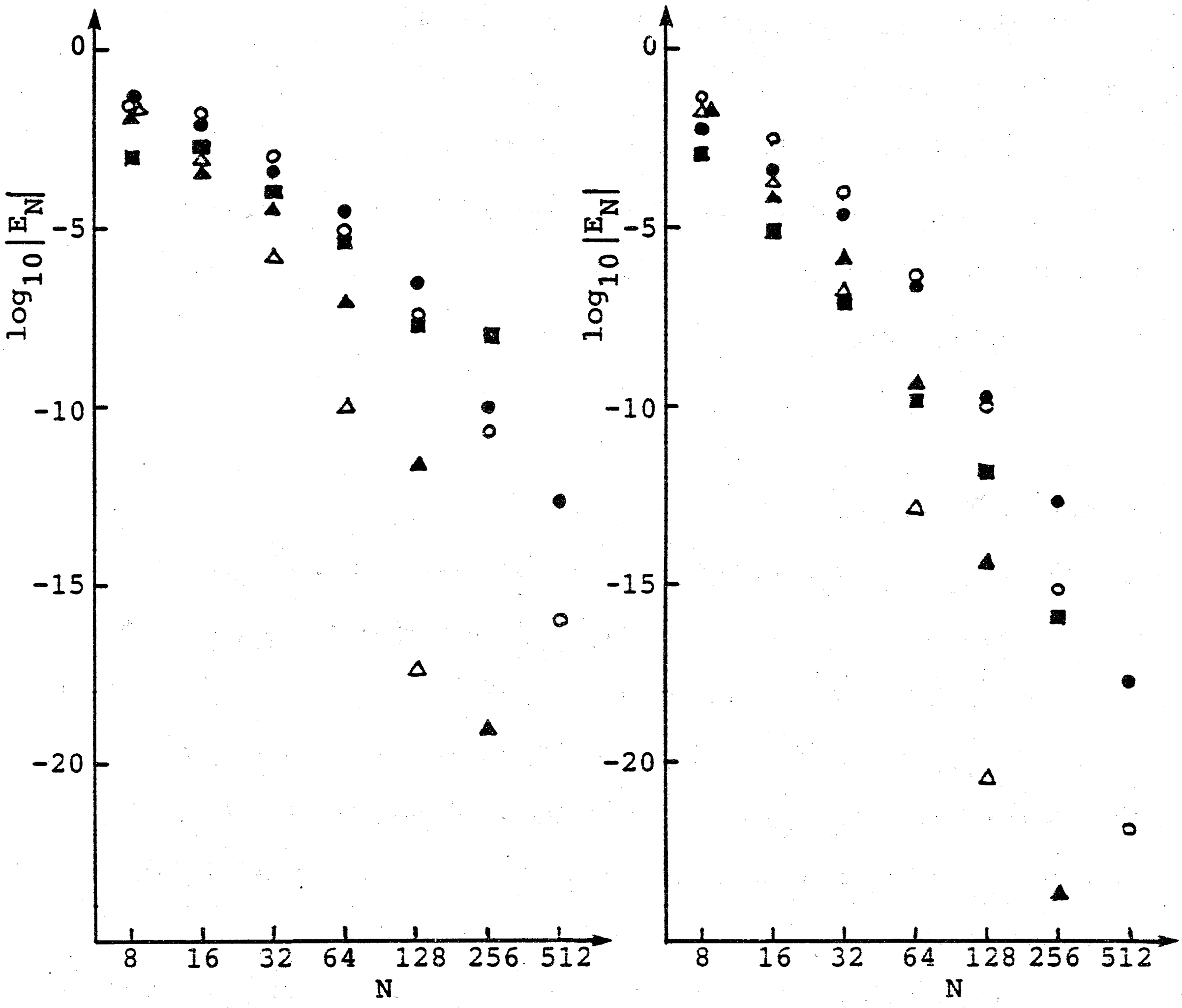
$$f_2(x) = \exp x, \qquad I = e-1 = 1.7182...,$$

$$f_3(x) = x^2, \qquad I = 1/3 = 0.3333...,$$

$$f_4(x) = 1/\sqrt{x}, \qquad I = 2,$$

$$f_5(x) = (\log x)/(x^2-1.5x+1.25), \qquad I = -1.0518...$$

$$f_6(x) = 2/(1+(2x-1)^2), \qquad I = \pi/2 = 1.5707... .$$



(1) Errors for $f_4(x) = 1/\sqrt{x}$

(2) Errors for $f_5(x) = \dfrac{\log x}{x^2-1.5x+1.25}$

Fig. 3.1. Numerical integration based on the transformation $x=\psi(t)$

○ : $\psi_{TANH}(t)$ ● : $\tilde{\psi}_{TANH}(t)$

△ : $\psi_{IMTDE}(t)$ ▲ : $\tilde{\psi}_{IMTDE}(t)$

■ : $\psi_U(t)$

The computations are done with mantissa of 28 hexadecimal digits by HITAC M-170H.

Fig. 3.1 illustrates the integration errors for $f_4(x)$ and $f_5(x)$ against the number of function evaluations. Similar results are obtained for other integrands. Note that (2.13) is verified.

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Appendix

We discuss the validity of the claim that

if $|\omega(\kappa)|$ decreases fast as $|\kappa|\to\infty$, then so does $|E_N(f)|$ as $N\to\infty$ for a well-behaved integrand f(x).

The following proposition, combined with (2.3), implies that the above claim holds true for polynomial integrands $f(x)=x^m$ in the particular case of $\psi(t)=\psi_{IMT}(t)$ (cf. (2.8)). Note that the proof is such that it can be adapted to other transformation functions $\psi(t)$ once bounds on $|\omega(\kappa)|$ and $|\omega'(\kappa)|$ are obtained.

Proposition A.1. Let $\psi(t)$ satisfy (2.1) and put

$$C_k = \int_0^1 \psi'(t)\exp(i2\pi kt)dt, \quad k\in Z, \tag{A.1}$$

$$D_k = \int_0^1 t\psi'(t)\exp(i2\pi kt)dt, \quad k\in Z, \tag{A.2}$$

$$C_k^m = \int_0^1 \psi(t)^m\psi'(t)\exp(i2\pi kt)dt, \quad k\in Z,\ m\in Z_+. \tag{A.3}$$

If

$$|C_k| \leq A\exp(-B\sqrt{|k|}), \quad k\in Z, \tag{A.4}$$

$$|D_k| \leq A\exp(-B\sqrt{|k|}), \quad k\in Z, \tag{A.5}$$

where A and B are constants independent of k, then

$$|C_k^m| \leq A_m|k| \exp(-B\sqrt{|k|}), \quad k\in Z\backslash\{0\}, \tag{A.6}$$

where A_m is defined by

$$A_0=A; \; A_{m+1} = A[3/2 + (m+1)(1+4/B^2)A_m/(2\pi)], \quad m=0,1,\ldots \tag{A.7}$$

Proof: Firstly, put

$$a_k^m = \int_0^1 (\psi(t)^m-t)\exp(i2\pi kt)dt, \quad k\in Z, \; m\in Z_+. \tag{A.8}$$

We have

$$a_0^1 = 0 \tag{A.9}$$

and

$$-1/2 \leq a_0^m \leq 0, \tag{A.10}$$

since

$$a_0^m = \int_0^1 (\psi(t)^m-t)dt = \int_0^1 \psi(t)^m dt - 1/2$$

and

$$0 \leq \int_0^1 \psi(t)^m dt \leq \int_0^1 \psi(t)dt = 1/2.$$

For $k\in Z\backslash\{0\}$, integration by parts yields

$$\begin{aligned} a_k^m &= [(\psi(t)^m-t)\exp(i2\pi kt)/(i2\pi k)]_{t=0}^1 \\ &\quad - \int_0^1 (m\psi(t)^{m-1}\psi'(t)-1)\exp(i2\pi kt)/(i2\pi k)dt \\ &= -(m/i2\pi k) \int_0^1 \psi(t)^{m-1}\psi'(t)\exp(i2\pi kt)dt \\ &= -(m/i2\pi k)\, C_k^{m-1}. \end{aligned} \tag{A.11}$$

Now we will establish (A.6) by induction with respect to m using the following identity:

$$C_k^{m+1} = D_k + a_0^{m+1}C_k - ((m+1)/i2\pi) \sum_{j\neq 0} C_j^m C_{k-j}/j, \tag{A.12}$$

which follows from

$$\begin{aligned} C_k^{m+1} &= \int_0^1 (\psi(t)^{m+1}-t)\psi'(t)\exp(i2\pi kt)dt + \int_0^1 t\psi'(t)\exp(i2\pi kt)dt \\ &= \sum_{j=-\infty}^{\infty} a_j^{m+1}C_{k-j} + D_k \end{aligned}$$

combined with (A.11).

Basis (m=0): (A.6) for m=0 is obvious from (A.1), since $C_k^0 = C_k$ and $A_0 = A$.

Induction: Suppose (A.6) holds true for m. From (A.12) follows

$$|C_k^{m+1}| \leq |D_k| + |a_0^{m+1}C_k| + ((m+1)/2\pi) \sum_{j\neq 0} |C_j^m C_{k-j}/j|. \qquad \text{(A.13)}$$

We have

$$|a_0^{m+1}C_k| \leq (A/2)\exp(-B\sqrt{|k|}) \qquad \text{(A.14)}$$

from (A.4) and (A.10). The last part of (A.13) is estimated as follows by (A.4) and (A.6):

$$\sum_{j\neq 0} |C_j^m C_{k-j}/j|$$

$$\leq \sum_{j\neq 0} A_m|j| \exp(-B\sqrt{|j|}) \cdot A\exp(-B\sqrt{|k-j|})/|j|$$

$$= A_m A \sum_{j\neq 0} \exp[-B(\sqrt{|j|}+\sqrt{|k-j|})]$$

$$= A_m A\Big(\sum_{j=1}^{|k|} \exp[-B(\sqrt{j}+\sqrt{|k|-j})] + 2\sum_{j=1}^{\infty} \exp[-B(\sqrt{j}+\sqrt{|k|+j})]\Big)$$

$$\leq A_m A(|k| + 4/B^2)\exp(-B\sqrt{|k|}), \qquad \text{(A.15)}$$

since

$$\sum_{j=1}^{|k|} \exp[-B(\sqrt{j}+\sqrt{|k|-j})] \leq \sum_{j=1}^{|k|} \exp(-B\sqrt{|k|}) = |k| \exp(-B\sqrt{|k|})$$

and

$$\sum_{j=1}^{\infty} \exp[-B(\sqrt{j}+\sqrt{|k|+j})]$$

$$\leq \exp(-B\sqrt{|k|}) \sum_{j=1}^{\infty} \exp(-B\sqrt{j})$$

$$\leq \exp(-B\sqrt{|k|}) \int_0^{\infty} \exp(-B\sqrt{x})dx = 2\exp(-B\sqrt{|k|})/B^2.$$

Substituting (A.5), (A.14) and (A.15) into (A.13), we obtain

$$|C_k^{m+1}| \leq A_{m+1}|k| \exp(-B\sqrt{|k|})$$

with A_{m+1} given by (A.7). Q.E.D.

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