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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

Kazuo Murota

Institute of Socio-Economic Planning, University of Tsukuba

筑波大　社会工学系　室田一雄

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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

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

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

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

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

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

and

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

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

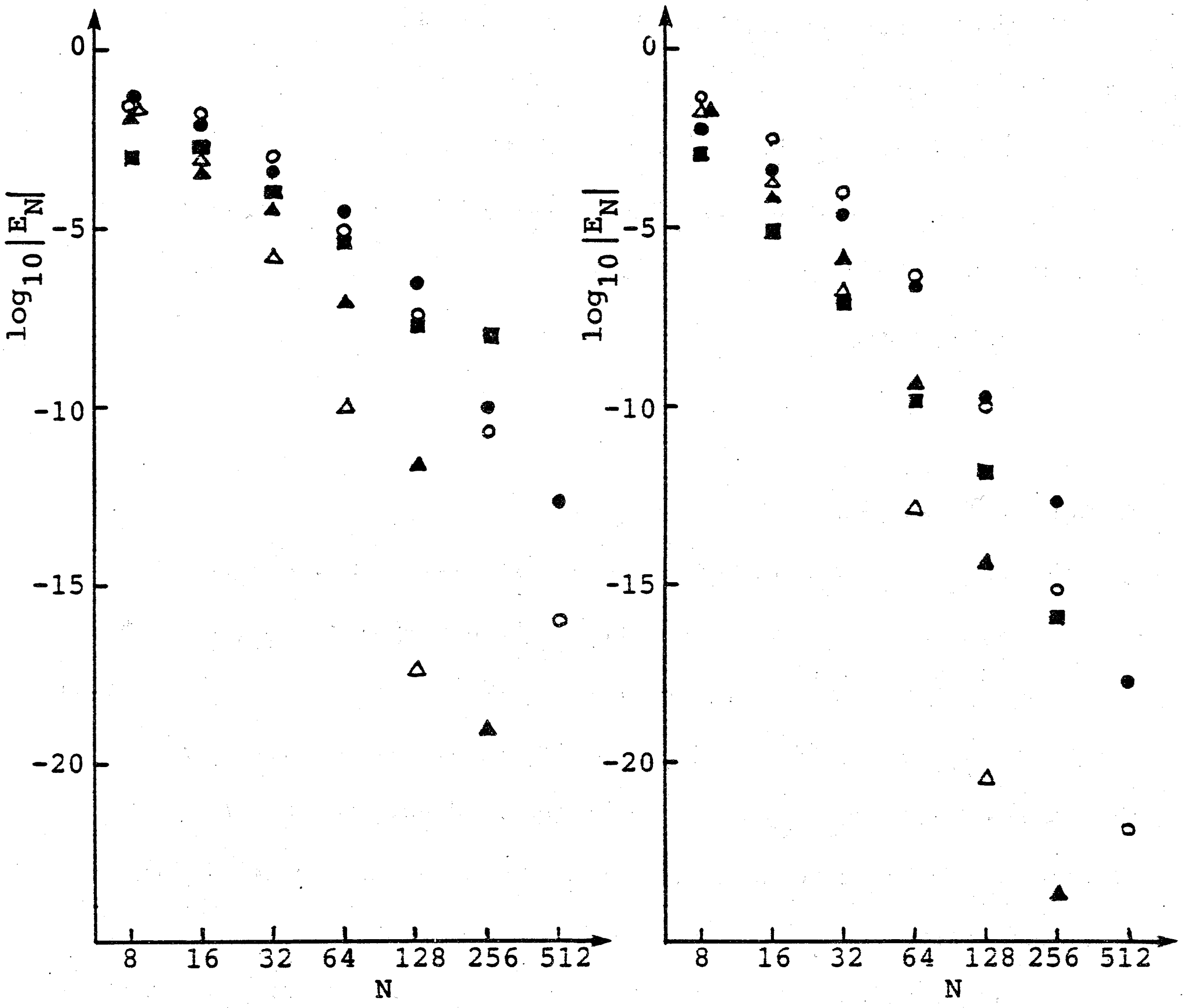
$$\psi_{TANH}(t) = (1/2)\tanh[(1/4)(1/(1-t)-1/t)] + 1/2, \qquad (3.1)$$

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

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:

$f_1(x) = 1,$	$I = 1,$
$f_2(x) = \exp x,$	$I = e-1 = 1.7182...,$
$f_3(x) = x^2,$	$I = 1/3 = 0.3333...,$
$f_4(x) = 1/\sqrt{x},$	$I = 2,$
$f_5(x) = (\log x)/(x^2-1.5x+1.25),$	$I = -1.0518...$
$f_6(x) = 2/(1+(2x-1)^2),$	$I = \pi/2 = 1.5707...\ .$



(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

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

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

where A and B are constants independent of k, then

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

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 $k \in Z \setminus \{0\}$, 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

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

We have

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

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

$$\begin{aligned}
&\sum_{j\neq 0} |C_j^m C_{k-j}/j| \\
&\leq \sum_{j\neq 0} A_m|j| \exp(-B\sqrt{|j|})\cdot A\exp(-B\sqrt{|k-j|})/|j| \\
&= A_m A \sum_{j\neq 0} \exp[-B(\sqrt{|j|}+\sqrt{|k-j|})] \\
&= A_m A\Big(\sum_{j=1}^{|k|} \exp[-B(\sqrt{j}+\sqrt{|k|-j})] + 2\sum_{j=1}^{\infty} \exp[-B(\sqrt{j}+\sqrt{|k|+j})] \Big) \\
&\leq A_m A(|k| + 4/B^2)\exp(-B\sqrt{|k|}),
\end{aligned} \tag{A.15}$$

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

$$\begin{aligned}
&\sum_{j=1}^{\infty} \exp[-B(\sqrt{j}+\sqrt{|k|+j})] \\
&\leq \exp(-B\sqrt{|k|}) \sum_{j=1}^{\infty} \exp(-B\sqrt{j}) \\
&\leq \exp(-B\sqrt{|k|}) \int_0^{\infty} \exp(-B\sqrt{x})dx = 2\exp(-B\sqrt{|k|}) / B^2.
\end{aligned}$$

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.

References

Davis, P.J., and P. Rabinowitz [1984]: Methods of Numerical Integration. 2nd ed., Academic Press.

Iri, M., and K. Kabaya [1985]: Sum of uniformly distributed random variables and a family of nonanalytic functions. Preprint.

Iri, M., S. Moriguti and Y. Takasawa [1970]: On a certain quadrature formula (in Japanese). Kokyuroku, Res. Inst. Math. Sci., Kyoto Univ., No.91, pp.82-118.

Mori, M. [1978]: An IMT-type double exponential formula for numerical integration. Publ. Res. Inst. Math. Sci., Kyoto Univ., Vol.14, pp.713-729.

Mori, M. [1985]: Quadrature formulas obtained by variable transformation and the DE-rule. J. Comput. Appl. Math., Vol.12&13, pp.119-130.

Murota, K., and M. Iri [1982]: Parameter tuning and repeated application of the IMT-type transformation in numerical quadrature. Numer. Math., Vol.38, pp.347-363.

Nishii, O., K. Murota and M. Iri [1985]: On a quadrature formula using a nonanalytic transformation of the integration variable (in Japanese). Presented at Res. Inst. Math. Sci., Kyoto Univ., on November 21, 1985. To appear in Kokyuroku (this volume), Res. Inst. Math. Sci., Kyoto Univ.

Takahasi, H., and Mori, M. [1973]: Quadrature formulas obtained by variable transformation. Numer. Math., Vol.21, pp.206-219.

Takahasi, H., and Mori, M. [1974]: Double exponential formulas for numerical integration. Publ. Res. Inst. Math. Sci., Kyoto Univ., Vol.9, pp.721-741.