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Parameter Tuning and Repeated Application of the IMT-type Transformation in Numerical Quadrature

Kazuo MUROTA*, Masao IRI*

Introduction

It has been recognized that the change of variable is one of the most powerful guiding principles in constructing a numerical quadrature formula which is both efficient (in the sense that the number of function evaluations is small) and robust against integrable end-point singularities. Among the quadrature formulas so far proposed are the IMT rule [5], the double exponential formulas [13] and the IMT-type double exponential formula [6]. Similar observations are made for multiple integrals in [8].

To be specific, the given integral

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

is transformed into

$$I = \int_\alpha^\beta f(\psi(t))\psi'(t)dt \tag{1.2}$$

through a suitable transformation $x = \psi(t)$. Here the interval of integration (α,β) may possibly be infinite, as is the case with the double exponential formula. Then the trapezoidal rule with equal mesh size h is applied to the transformed integral (1.2) to yield an approximation to I:

$$S_h = h \sum_j w_j^{(h)} f(x_j^{(h)}). \tag{1.3}$$

When the transformed interval of integration (α,β) is infinite, the right-hand side involves an infinite number of terms, which should be

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* Department of Mathematical Engineering and Instrumentation Physics, Faculty of Engineering, University of Tokyo, Bunkyo-ku, Tokyo, Japan 113.

trimmed to a finite number n without impairing the accuracy. In general, if some of the summands on the right-hand side are neglected, the remaining number n is called the "effective number" of sampling points. On the other hand, in the case of a finite interval (α,β), $N = (\beta-\alpha)/h$ is referred to as the "degree" of a quadrature formula.

The error induced in the process of discretization by the trapezoidal rule is termed the "discretization error", in contrast to the error which may be introduced when the sum (1.3) is replaced by that with a smaller number of terms. The latter is called here the "trimming error", though it was named the truncation error in [13]. (Truncation error sometimes means the same thing as discretization error!) The discretization error for a constant integrand is called the "intrinsic error" of the formula, and is known to well represent the performance of a quadrature formula of this kind for regular integrands.

The IMT rule [1], [2], [3], [5], [11] employs the following transformation, called the IMT transformation,

$$\psi^{\mathrm{IMT}}(t) = \frac{1}{Q}\int_0^t \exp[-(\frac{1}{t} + \frac{1}{1-t})]\,dt$$
$$Q = \int_0^1 \exp[-(\frac{1}{t} + \frac{1}{1-t})]\,dt \tag{1.4}$$

which maps the unit interval onto itself. The error is due solely to the discretization by the trapezoidal rule and behaves itself as $\exp(-c\sqrt{N})$ asymptotically, where N is the degree of the formula (=the nominal number of function evaluations). The transformation

$$\psi^{\mathrm{TANH}}(t) = \frac{1}{2}\tanh[-\frac{1}{2}(\frac{1}{t} - \frac{1}{1-t})] + \frac{1}{2}\ , \tag{1.5}$$

which we call the TANH transformation, would be a possible alternative by which to map the unit interval onto itself.

The double exponential formula [13], on the other hand, converts the integral over the unit interval into that over the infinite interval by means of the transformation function

$$\psi^{DE}(t) = \frac{1}{2}\tanh\left(\frac{\pi}{2}\sinh t\right) + \frac{1}{2}, \tag{1.6}$$

which will be called the DE (standing for Double Exponential) transformation. The error, due both to discretization and to trimming, is estimated asymptotically as* $\exp(-cn/\log n)$, where n is the "effective number" of function evaluations. The transformed integrand in (1.2) in this case decays like the double exponential function as $|t| \to \infty$. There may be a variety of potential candidates for the transformation function which yield different decay rates of the transformed integrand [4], [12]. But, in [13], the double exponential decay is claimed to be optimal when the transformed interval is infinite. This fact has also been observed in the numerical experiment in [9], where it is shown that the triple or quadruple exponential transformation is inferior to the double. The optimality of the constant $\pi/2$ in ψ^{DE} above was reported by Mori.**

In this paper, the IMT transformation is generalized to obtain better quadrature formulas. In the first place, two parameters are introduced in the IMT transformation.*** The asymptotic error estimate for the parameterized IMT rule is obtained in an analogous manner to that for the original IMT rule. The error estimate suggests a pronounced improvement in the efficiency of the quadrature formula, to the extent that the IMT rule with tuned parameters can

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* The relation to Stenger's lower bound [10] is discussed in Appendix.

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*** Numerical study of the parameterized IMT rule is reported also in [3].

compete with the double exponential formula at least for practical purposes. Another direction of generalization is to apply the parameterized IMT transformation repeatedly, which is possible since it maps the unit interval onto itself. Asymptotic error estimate, as well as numerical study, shows that, as opposed to the case of the infinite interval, the double exponential decay is not optimal in a finite interval. Repeated application of the IMT transformation leads to quadrature formulas which are more efficient in the asymptotic sense, though the numerical experiment shows that the efficiency is rather insensitive to the number of repetitions of the IMT transformation. It is remarked that the IMT-type double exponential formula by Mori [6] may be regarded as a formula obtained by the repeated application of the TANH transformation ψ^{TANH}, and its possible generalization is also discussed.

1. Parameterization of the IMT transformation

Two parameters $a(>0)$ and $p(>0)$ are introduced in the IMT transformation (1.4):

$$\begin{aligned} \psi^{\mathrm{IMT}}_{a,p}(t) &= \frac{1}{Q(a,p)} \int_0^t \exp[-a(\frac{1}{t^p} + \frac{1}{(1-t)^p})]\, dt, \\ Q(a,p) &= \int_0^1 \exp[-a(\frac{1}{t^p} + \frac{1}{(1-t)^p})]\, dt . \end{aligned} \tag{2.1}$$

The resulting family of quadrature formulas will be called the IMT-Single(a,p) rule. The IMT-Single(1,1) rule is nothing but the original IMT rule.

By the saddle point method, the asymptotic estimate for the intrinsic error of the formula of degree N is derived [7]:

$$\varepsilon \sim 2^{\frac{p+5}{2}} (\frac{ap}{2\pi N})^{\frac{p+2}{2(p+1)}} \exp[-a^{\frac{1}{p+1}}(p+1)(\frac{2\pi N}{p})^{\frac{p}{p+1}} \sin\frac{\pi}{2(p+1)} + a(2^{p+1}-1)]. \tag{2.2}$$

The formula of degree N apparently requires N-1 function evaluations at N-1 sampling points, but part of them may be omitted without impairing the accuracy. The effective number n of sampling points is asymptotically estimated as

$$n \sim N[1 - 2 \left(\frac{2}{\pi}\right)^{\frac{1}{p}} \left(\frac{ap}{2\pi N}\right)^{\frac{1}{p+1}}] \tag{2.3}$$

for constant integrands [7].

As is shown in Table 1, the asymptotic estimates (2.2) and (2.3) are in good agreement with the observations made in numerical experiments, though the agreement is expected to become the poorer the larger the parameters a and p are.

Table 1. Errors of the IMT-Single rule for $\int_0^1 \frac{1}{2}\,dx$

Degree N	IMT-Single(1,1)				IMT-Single(10,1)			
	Error*		Points		Error*		Points	
	Obs.	Est.	Obs.	Est.	Obs.	Est.	Obs.	Est.
4	-2.6	-2.3	3	3	-0.4	+2.5	3	1
8	-4.5	-4.1	7	7	-1.8	-1.4	5	4
16	-5.5	-5.5	15	14	-8.7	-6.6	9	10
32	-8.4	-8.4	29	29	-15.3	-15.3	23	23
64	-12.5	-12.6	61	60	-27.8	-26.2	51	51
128	-17.4	-17.4	123	122	/	-42.7	/	109
256	-25.4	-25.5	247	248	/	-66.6	/	230

Degree N	IMT-Single(1,2)				IMT-Single(0.4,3)			
	Error*		Points		Error*		Points	
	Obs.	Est.	Obs.	Est.	Obs.	Est.	Obs.	Est.
4	-0.7	-0.2	3	1	-0.4	+0.4	3	1
8	-2.7	-3.1	5	4	-2.0	-1.6	5	3
16	-6.7	-6.4	9	9	-5.0	-5.1	7	7
32	-11.5	-11.4	21	21	-10.2	-10.1	17	17
64	-20.3	-20.0	47	47	-18.8	-18.7	39	38
128	/	-33.6	/	100	/	-33.2	/	85
256	/	-54.2	/	212	/	-57.9	/	183

* Errors in $\log_{10}|\text{absolute error}|$

Obs.: Observed by experiments; Est.: Estimated by asymptotic formulas

The error ε and the effective number n of sampling points are implicitly related by (2.2) and (2.3) for a formula of degree N with parameter (a,p). In order to grasp the relation intuitively, we draw contour lines of ε and n on the plane, for a fixed p, with abscissa N and ordinate a, as shown in Fig. 1, where p=1. When we need the accuracy of 10^{-6}, for instance, we can choose, among the formulas with p=1, those formulas with a and N lying on the contour line of $\varepsilon=10^{-6}$. The optimal formula, i.e., the formula with the least effective number n, with p=1 for $\varepsilon=10^{-6}$, is approximately found to be the formula of degree N=14 with a=8.

The optimal formulas for different requests of accuracy are indicated by a broken line. Thus no uniformly optimal set of parameters exists. It is also observed that the efficiency strongly depends on the parameters, especially for a small.

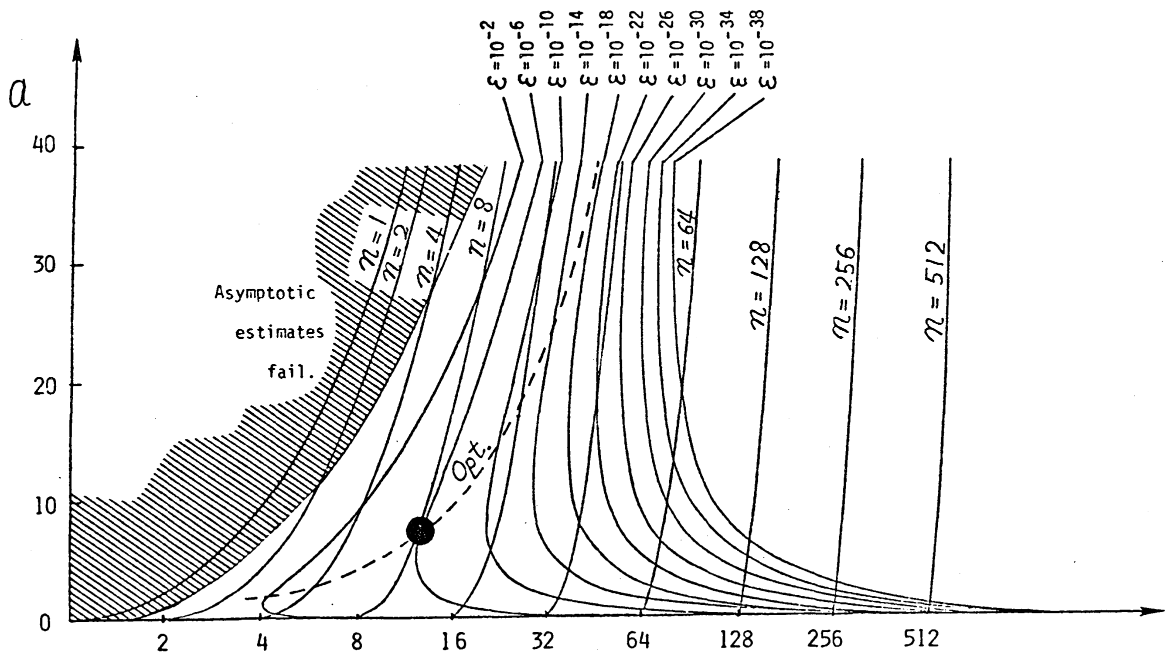

Fig. 1. Contour map of ε and n for IMT-Single with $p=1$

The TANH transformation (1.5) can also be parameterized as

$$\psi_{a,p}^{TANH}(t) = \frac{1}{2}\tanh\left[-\frac{a}{2}\left(\frac{1}{t^p} - \frac{1}{(1-t)^p}\right)\right] + \frac{1}{2}. \tag{2.4}$$

The corresponding quadrature rule, to be called the TANH-Single(a,p) rule, or simply the TANH(a,p) rule, behaves itself quite similarly to the IMT-Single(a,p) rule when a is small, while, for a large, it is significantly inferior to the IMT-Single(a,p) rule. This is due to the fact that, as depicted in Fig. 2, the parameterized TANH transformation (2.4) possesses an infinite number of extraneous poles, some of which are located close to the real axis at the middle of the interval of integration when a is large. Note that the parameterized IMT transformation (2.1) has no singularities except those at the ends of the interval of integration.

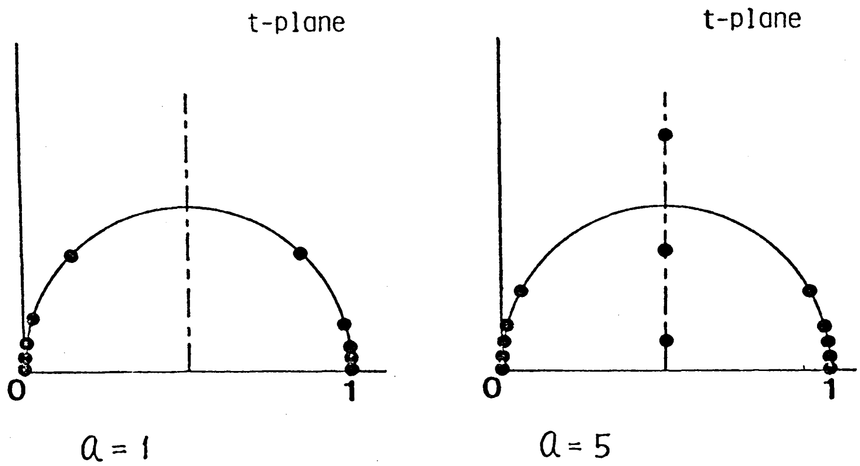

Fig. 2. Singularities of TANH transformation $\psi_{a,1}^{TANH}(t)$

2. Repetition of the IMT transformation

Repeated application of the parameterized IMT transformation leads to a further extension of the IMT rule. That is, the composite $\psi^{\mathrm{IMT}}_{a_1,p_1} \circ \psi^{\mathrm{IMT}}_{a_2,p_2}$ of the IMT tarnsformation functions may be considered as a transformation function ψ in (1.2). The family of quadrature formulas thus obtained will be called the IMT-Double$(a_1,p_1;a_2,p_2)$ rule.

The error of the IMT-Double$(a_1,p_1;a_2,p_2)$ rule of degree N is asymptotically estimated [7] as

$$\exp\left(-\frac{c\,N}{(\log N)^{1+1/p_2}}\right),$$

where c is a positive constant depending on the parameters. This estimate implies that the second transformation $\psi^{\mathrm{IMT}}_{a_2,p_2}$ is asymptotically of dominant importance, though, in the range of practical interest, the numerical experiment points to the contrary, as will be shown later.

The IMT-type double exponential formula [6], originally designed to simulate the double exponential decay in a finite interval, can be viewed as the quadrature formula resulting from the repeated application of the TANH transformation: $\psi = \psi^{\mathrm{TANH}}_{\pi/2,1} \circ \psi^{\mathrm{TANH}}_{\pi/4,1}$.

The fact that the composition of the IMT transformation favors the efficiency of the quadrature formula seems to suggest that further improvement will be brought about by the repeated change of the variable of integration through the IMT transformation. The quadrature formula with $\psi = \psi^{\mathrm{IMT}}_{a_1,p_1} \circ \psi^{\mathrm{IMT}}_{a_2,p_2} \circ \psi^{\mathrm{IMT}}_{a_3,p_3}$ will be called the IMT-Triple$(a_1,p_1;a_2,p_2;a_3,p_3)$ rule. The formula with $\psi = \psi^{\mathrm{IMT}}_{a_1,p_1} \circ \psi^{\mathrm{IMT}}_{a_2,p_2} \circ \psi^{\mathrm{IMT}}_{a_3,p_3} \circ \psi^{\mathrm{IMT}}_{a_4,p_4}$ will be called the IMT-Quadruple $(a_1,p_1;a_2,p_2;a_3,p_3;a_4,p_4)$ rule, and so forth.

The asymptotic error estimates for the quadrature formulas of degree N obtained from the repeated application of $\psi_{1,1}^{\mathrm{IMT}}$ are given by

IMT-Single rule: $\exp(-c\sqrt{N})$

IMT-Double rule: $\exp\left(-\dfrac{c\,N}{(\log N)^2}\right)$

IMT-Triple rule: $\exp\left(-\dfrac{c\,N}{(\log N)(\log\log N)^2}\right)$

IMT-Quadruple rule: $\exp\left(-\dfrac{c\,N}{(\log N)(\log\log N)(\log\log\log N)^2}\right)$.

Though these estimates are not claimed to be of practical value, they suggest that the double exponential decay, which is realized by the IMT-Double rule, is not optimal, and that the repeated change of the variable of integration will result in an improvement, at least asymptotically. It is also seen that none of these formulas can outperform the double exponential formula in the asymptotic sense, where the asymptotic error estimate for the latter is given by $\exp(-cn/\log n)$.

3. Numerical study

Before presenting the numerical results, a comment is made on what is the practical measure of efficiency of a quadrature formula when used as an automatic integrator. When given necessary input data such as the integrand function and the requested accuracy, an automatic integrator based on an iterative scheme would continue computing successive approximations until it is convinced to have achieved the requested accuracy. Thus it should evaluate a larger number of function values than is really necessary before it returns an answer with confidence.

For a particular choice of initial mesh size h_0, the relation between the requested accuracy and the number of function evaluations looks like a "staircase" consisting of solid circles in Fig. 3. The corresponding sequence of hollow circles representing the relation between the achieved accuracy and the number of function evaluations also forms another "staircase". These staircases slide like an escalator within the region bounded by the upper and the lower envelope, depending on the initial mesh size h_0, the optimal value of which cannot practically be found before the computation. Note that the lower envelope of the "solid staircase" agrees approximately with the upper envelope of the "hollow staircase".

From the practical point of view, the relation of the number of sampling points to the requested accuracy is more significant than that to the achieved accuracy. The upper envelope of the staircase-like relation between the requested accuracy and the number of

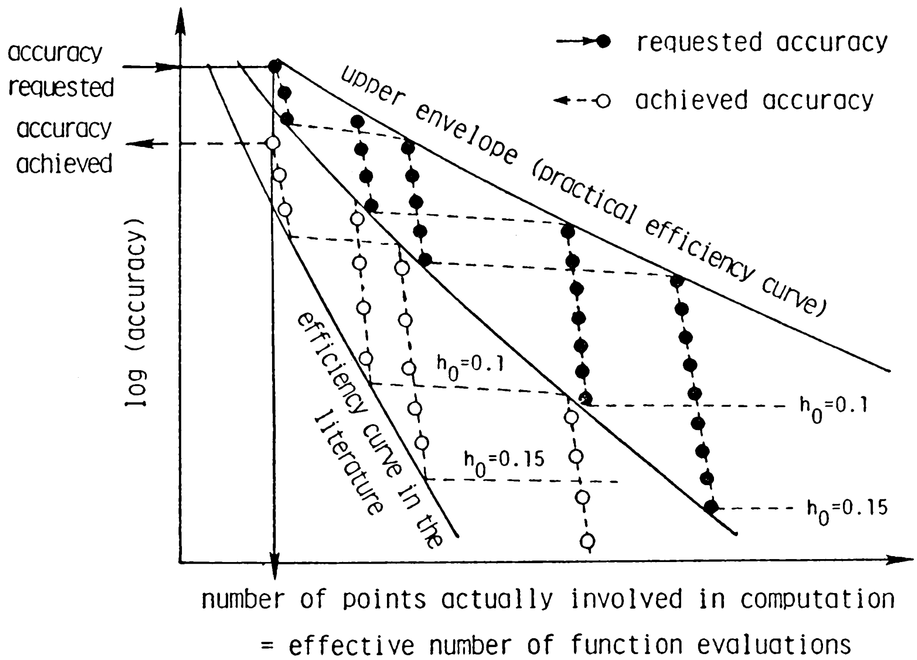

Fig. 3. Measure of efficiency of an automatic integrator

sampling points is adopted here as the relevant line representing the efficiency of the automatic integrator, though, usually in the literature, the lower envelope of the relation between the achieved accuracy and the number of sampling points has been used [6], [9], [12], [13].

Intrinsic errors of several quadrature formulas are shown in Figs. 4 to 9 in terms of the efficiency curve mentioned above. The original IMT rule, the double exponential formula and the IMT-type double exponential formula are compared in Fig. 4. The parameter tuning of the IMT-Single(a,p) rule enhances the efficiency to a considerable degree; (a,p) = (10,1) is fairly good (Fig. 5). The TANH-Single(a,p) rule is inferior to the IMT-Single(a,p) rule when p=1 and a is large (Fig. 6), as has already been explained. (For p=1, the optimal choice of a for TANH-Single(a,p) rule is $a \doteqdot 3$.) In Fig. 7, formulas of the IMT-Double(a_1,p_1;a_2,p_2) rule with different parameters are compared. The first transformation $\psi^{\mathrm{IMT}}_{a_1,p_1}$ of $\psi^{\mathrm{IMT}}_{a_1,p_1} \circ \psi^{\mathrm{IMT}}_{a_2,p_2}$ is influential, as opposed to the theoretical asymptotic estimate. The parameter dependence is not so conspicuous for the IMT-Double rule as for the IMT-Single rule. The IMT-type double exponential formula can be improved considerably by introducing parameters and tuning them (Fig. 8). The triple repetition of the transformation does not deteriorate the efficiency (Fig. 9); compare the IMT-Triple(1,2;1,1;1,1) rule in Fig. 9 with the IMT-Double(1,2;1,1) rule in Fig. 7. This means that the IMT-Double rule does an excellent job even when it is applied to a function with an exponential decay before the transformation. In other words, the quadrature formula of this kind is robust not only against bad, or singular, integrands but also against well-behaved integrands.

The algebraic singularities (Fig. 10) and the logarithmic singularity (Fig. 11) can be successfully dealt with by these formulas. Repeated application of the transformation results in the robustness against end-point singularities.

4. Conclusion

Introduction of parameters in the IMT transformation and its repeated application with tuned parameters enhance the efficiency of the resulting quadrature formulas to the extent that they can compete with the double exponential formula at least in the range of practical interest.

In the case where the integrals are transformed to those over a finite interval as in the IMT rule, there is no particular reason for insisting on the superiority of the double exponential decay in the neighborhood of the end-points; repeated application of the IMT transformation does no harm.

The IMT-type double exponential formula by Mori can be improved by selecting better parameters of the transformation.

Acknowledgement

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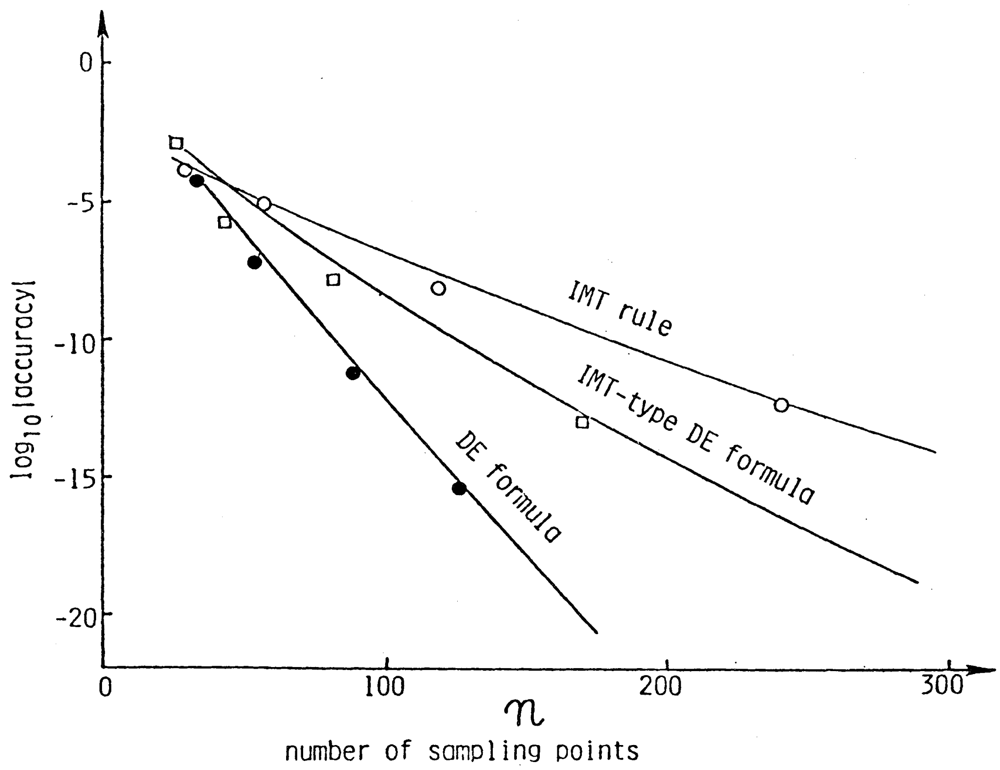


Fig. 4. Intrinsic error of the existing formulas

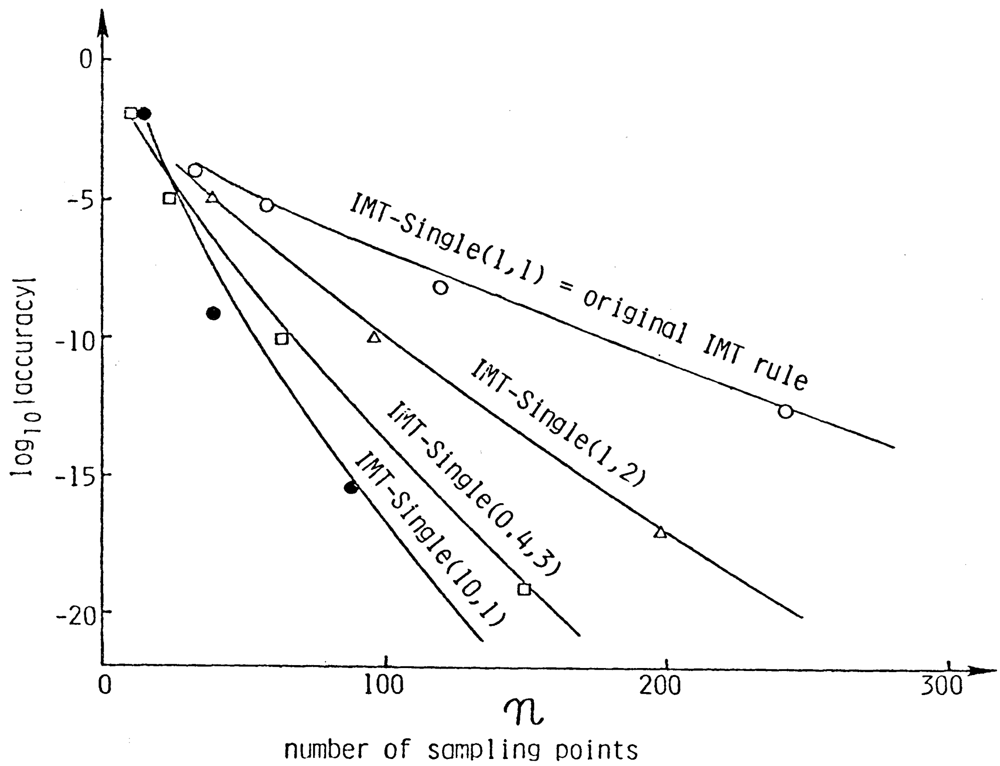


Fig. 5. Intrinsic error of the IMT-Single rule

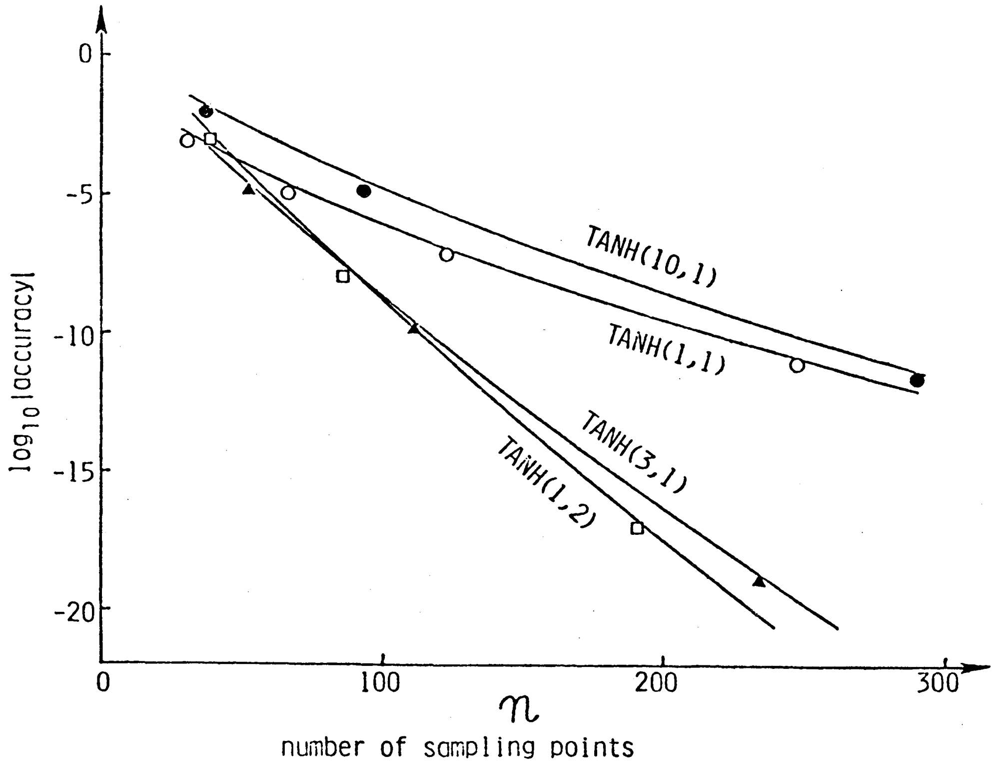


Fig. 6. Intrinsic error of the TANH-Single rule

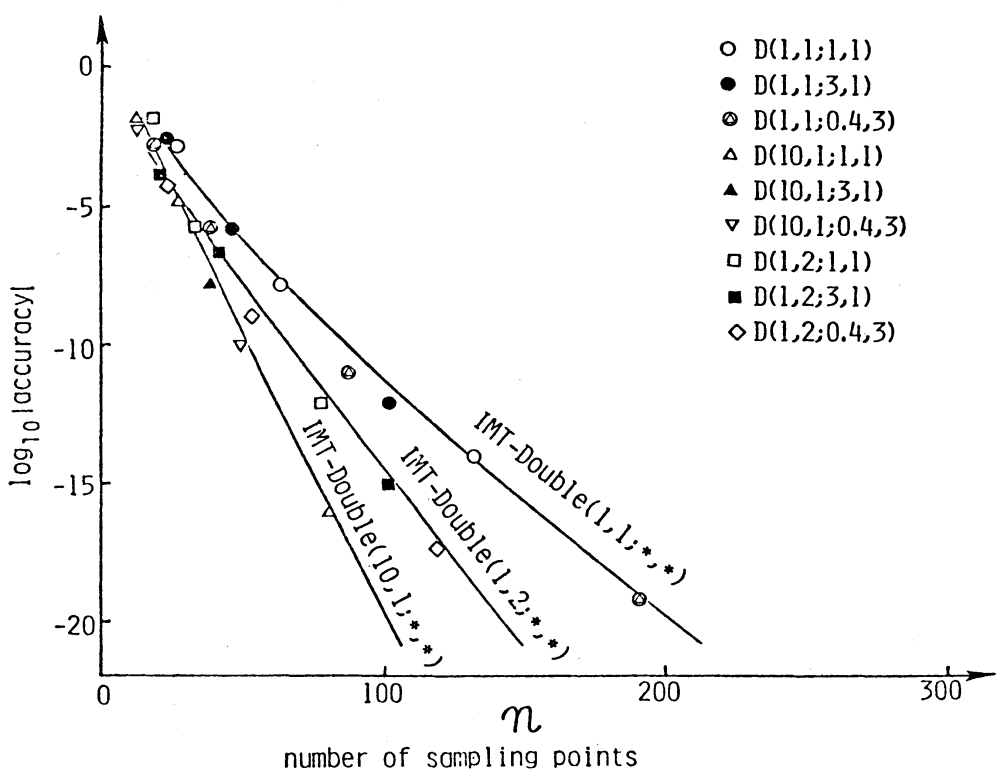


Fig. 7. Intrinsic error of the IMT-Double rule

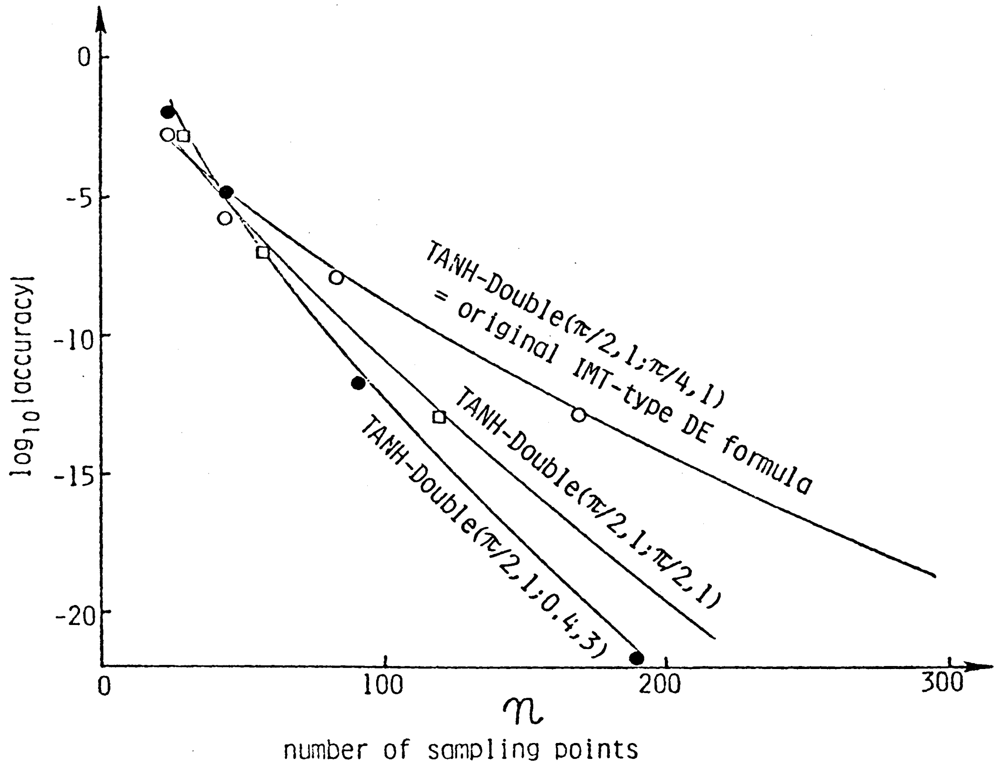


Fig. 8. Intrinsic error of the IMT-type double exponential formula

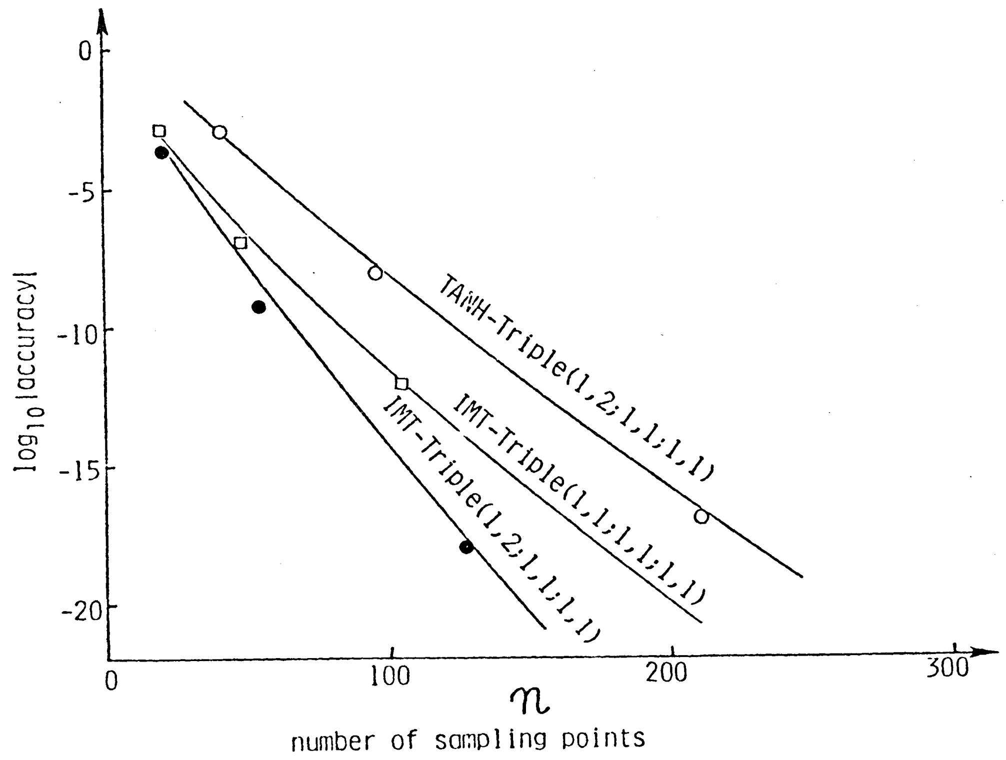


Fig. 9. Intrinsic error of the formulas with triple transformation

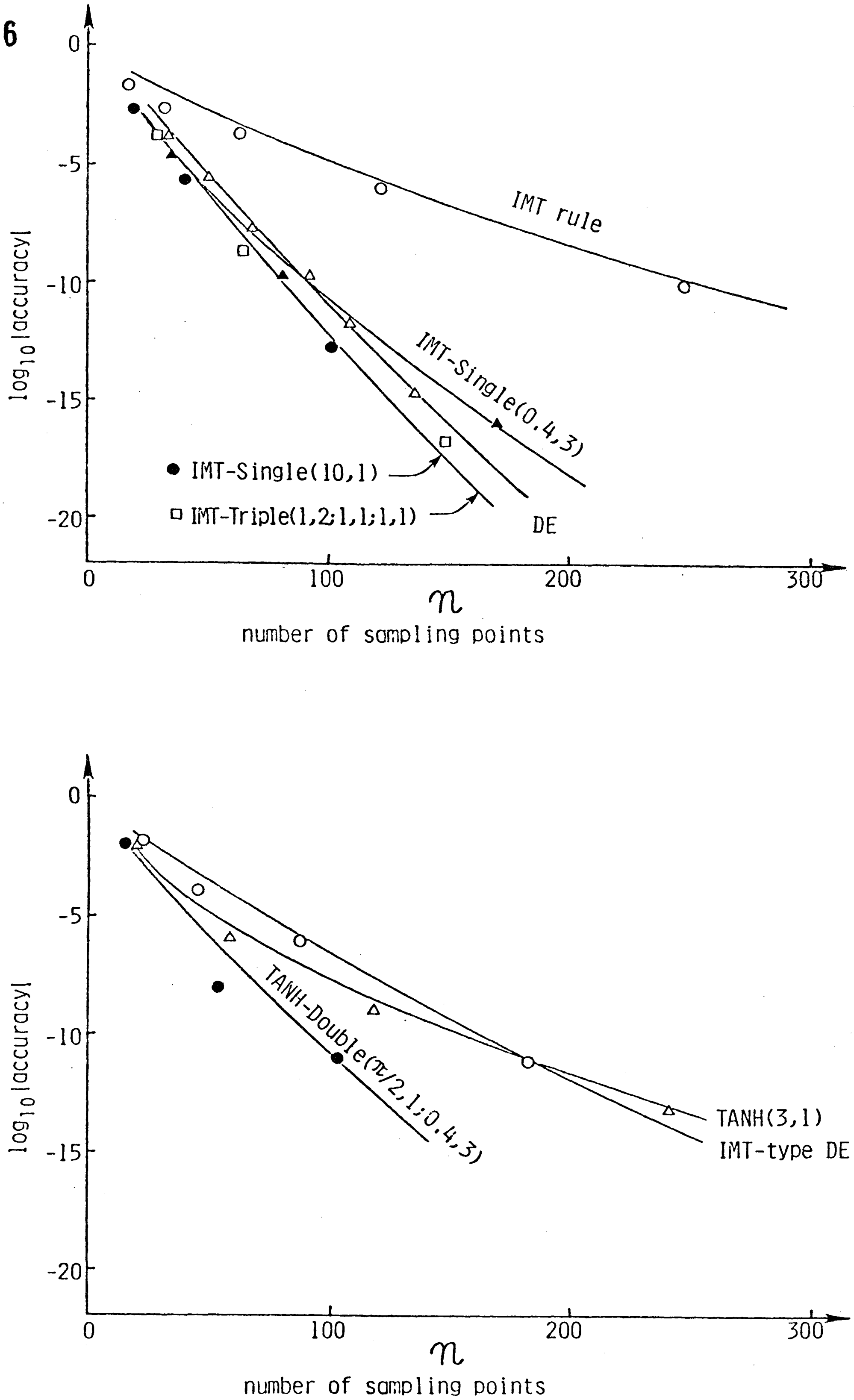
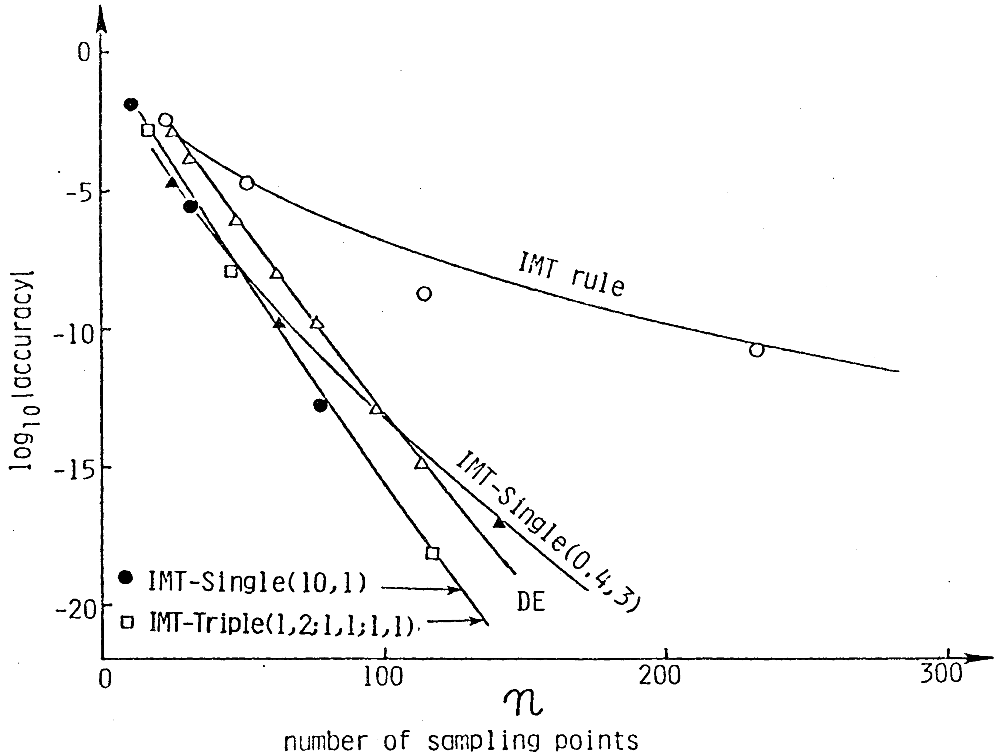


Fig. 10. Integration of $\int_0^1 \left(\frac{1}{\sqrt{X}} + \frac{1}{\sqrt{1-X}}\right) dX$



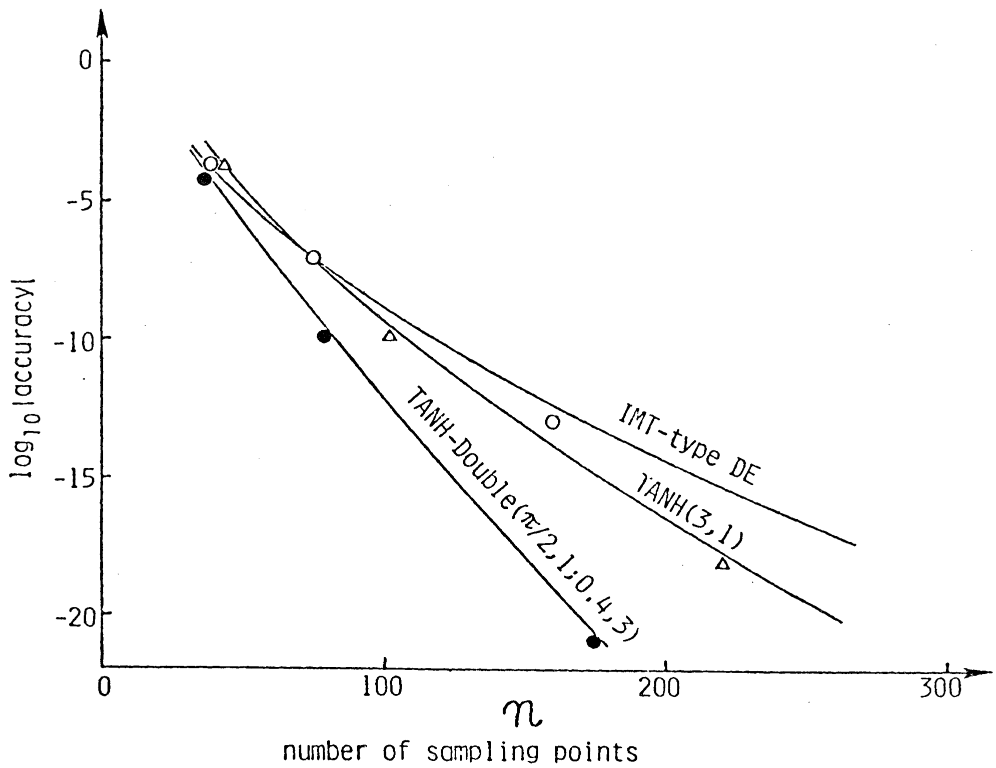


Fig. 11. Integration of $\int_0^1 \log X \, dX$

Appendix. A comment on Stenger's lower bound

F. Stenger [10] gives a lower bound for the possible asymptotic behavior of the errors involved in a quadrature scheme. Theorem 1.1 in that paper states that, for any $\varepsilon>0$, there exists an integer $n(\varepsilon)\geq 0$ such that for all $n>n(\varepsilon)$

$$\inf_{x_j, w_j} \sup_{\substack{f\in H_p(U) \\ \|f\|_p=1}} \left|\int_{-1}^{1} f(x)dx - \sum_{j=1}^{n} w_j f(x_j)\right| \geq \exp[-(\sqrt{5}\pi+\varepsilon)\sqrt{n}],$$

where $H_p(U)$ denotes the family of all functions f that are analytic in the unit disc U such that

$$\|f\|_p = \lim_{r\to 1^-} \frac{1}{2\pi}\left(\int_0^{2\pi} |f(r\exp(i\theta))|^p d\theta\right)^{1/p} < \infty.$$

This theorem implies that for any quadrature formula with n function evaluations, there exists an "unfavorable" function f_n, depending on n, for which the quadrature formula gives a "poor" approximation with "relative" error larger than $\exp[-(\sqrt{5}\pi+\varepsilon)\sqrt{n}]$. But this theorem says nothing about the asymptotic behavior of the error when an integrand function is kept fixed and the number of function evaluations is increased. Thus, the theorem does not contradict the asymptotic error estimates in the present paper such as $\exp(-c\,n^{p/(p+1)})$, $\exp(-cn/\log n)$, etc.

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