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The double exponential formula for oscillatory functions over the half infinite interval

Takuya Ooura *

Department of Physics, Faculty of Science, Nagoya University, Hurou-cho, Chikusa-ku, Nagoya, 464, Japan

Masatake Mori

Department of Applied Physics, Faculty of Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113, Japan

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Abstract

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The double exponential formula is known to be very powerful for evaluation of various kinds of integrals, in particular integrals with end point singularities or integrals over the half infinite interval. It is also known that a weak point of this formula is the inefficiency when applied to a slowly decaying oscillatory integral over the half infinite interval such as $I = \int_0^\infty f_1(x) \sin x \, dx$, $f_1(x)$ is an algebraic function. In this paper we propose a new type of the double exponential formula which is quite efficient for evaluation of the integral mentioned above. It is based on such a transformation that makes the points of the formula after the transformation approach to the zeros of $\sin x$ double exponentially for large x.

Keywords: Numerical integration, variable transformation, double exponential formula, DE-transformation, oscillatory integral.

1. The double exponential formula for oscillatory integrals over the half infinite interval

The double exponential formula [6] (abbreviated as the DE-formula) can evaluate integrals with end point singularity or integrals over the half infinite interval efficiently, which conventional quadrature formulas cannot. However, there is a class of integrals that the DE-formula

* Present address: c/o M. Mori, Department of Applied Physics, Faculty of Engineering, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo, 113, Japan.

fails to integrate. They are integrals over the half infinite interval of a slowly decaying oscillatory function such as

$$I = \int_0^\infty f_1(x) \sin x \, \mathrm{d}x, \quad f_1(x) \text{ is a slowly decaying algebraic function.} \tag{1}$$

There are several remedies for this situation. The application of the Richardson's extrapolation method to the integral together with the DE-transformation is known to remarkably improve the situation [2,4,7]. In the present paper we propose a more efficient method for such kind of integrals which uses a new kind of DE-transformation.

Let the given integral be

$$I = \int_0^\infty f(x) \, \mathrm{d}x, \tag{2}$$

in which the integrand is such that

$$f(n\lambda + \theta) = 0, \quad \text{for large integer } n, \tag{3}$$

where λ and θ are some constants. This means that $f(x)$ has an infinite number of zeros with period λ for large x. The phase of the zeros may be shifted by θ with respect to the origin. If $f(x) = f_1(x) \sin \omega x$, then $\lambda = \pi/\omega$ and $\theta = 0$, while if $f(x) = f_1(x) \cos \omega x$, then $\lambda = \pi/\omega$ and $\theta = \pi/(2\omega)$.

Then we make a variable transformation

$$x = M\phi(t), \quad \phi(-\infty) = 0, \ \phi(+\infty) = \infty, \tag{4}$$

in (2) giving

$$I = \int_{-\infty}^\infty f(M\phi(t)) M\phi'(t) \, \mathrm{d}t, \tag{5}$$

where M is some large positive constant. Next we apply the trapezoidal rule with the constant shift θ/M to this integral which leads to

$$I_h = Mh \sum_{n=-\infty}^{\infty} f\left(M\phi\left(nh + \frac{\theta}{M}\right)\right) \phi'\left(nh + \frac{\theta}{M}\right). \tag{6}$$

Here we choose such $\phi(t)$ that

$$\phi(t) \sim t, \quad t \to +\infty, \tag{7}$$

i.e., that $M\phi(nh + \theta/M)$ approaches to $Mnh + \theta$ when $n \to \infty$, and that

$$\phi'(t) \sim 0, \quad t \to -\infty. \tag{8}$$

Moreover we employ a mesh size h satisfying

$$Mh = \lambda. \tag{9}$$

Then we have

$$f\left(M\phi\left(nh + \frac{\theta}{M}\right)\right) \simeq f(Mnh + \theta) = f(n\lambda + \theta) = 0, \quad h = \frac{\lambda}{M}, \tag{10}$$

from (3) for large n, so that we can truncate the summation I_h at some moderate positive n as far as $\phi(t)$ approaches to t rapidly. For large negative n we can truncate the summation by (8).

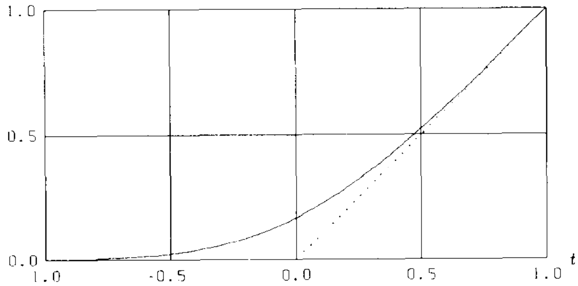

Fig. 1. The graph of $\phi(t)=t/\{1-\exp(-6\sinh t)\}$.

A typical and useful example of such kind of transformations is given by

$$\phi(t)=\frac{t}{1-\exp(-K\sinh t)}, \tag{11}$$

where K is some positive constant. The derivative is given by

$$\phi'(t)=\frac{1-(1+Kt\cosh t)\exp(-K\sinh t)}{(1-\exp(-K\sinh t))^2}. \tag{12}$$

As $t\to-\infty$, 0 or $+\infty$, $\phi(t)$ and $\phi'(t)$ behave as follows:

$$\phi(t)\sim\begin{cases}|t|\exp(-\frac{1}{2}K\exp|t|)\sim 0, & t\to-\infty,\\ \dfrac{1}{K}, & t\to 0,\\ t+t\exp(-\frac{1}{2}K\exp t)\sim t, & t\to+\infty,\end{cases} \tag{13}$$

$$\phi'(t)\sim\begin{cases}\frac{1}{2}K|t|\exp|t|\exp(-\frac{1}{2}K\exp|t|)\sim 0, & t\to-\infty,\\ \frac{1}{2}, & t\to 0,\\ 1, & t\to+\infty.\end{cases} \tag{14}$$

In other words, the derivative $\phi'(t)$ approaches to 0 double exponentially as $t\to-\infty$, while the function $\phi(t)$ itself approaches to t double exponentially as $t\to+\infty$. Note that when we write an integrator based on this transformation, we must be careful so that the numerical evaluation of $\phi(t)$ and $\phi'(t)$ in the neighborhood of $t=0$ does not give rise to the loss of significant digits.

In Fig. 1 we show the graph of $\phi(t)$ in the case of $K=6$.

2. Error analysis

As an example we evaluate the integral

$$I=\int_0^\infty\frac{\cos x}{1+x^2}\,dx=\frac{\pi}{2e} \tag{15}$$

by the formula based on the transformation

$$x=M\phi(t),\quad \phi(t)=\frac{t}{1-\exp(-6\sinh t)}. \tag{16}$$

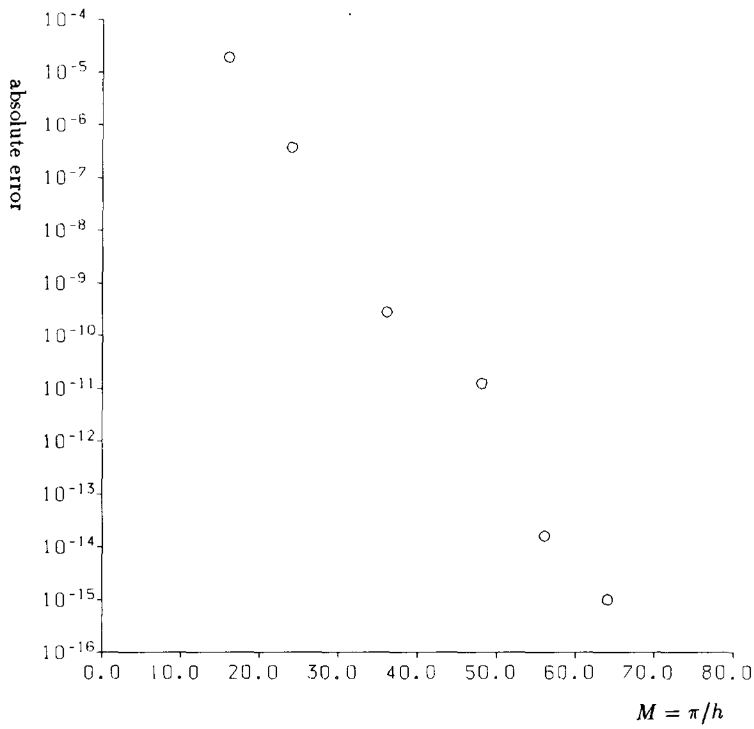

Fig. 2. The absolute error of the numerical integration of $\int_0^\infty \cos x/(1+x^2)\,dx = \pi/2e$ by the formula based on (16).

Figure 2 shows the absolute error of the result. The abscissa is $M=\pi/h$ and the ordinate is the error in logarithmic scale. From this graph we see that the absolute error behaves approximately as

$$\Delta I_h = I - I_h \sim \exp\left(-\frac{c}{h}\right), \tag{17}$$

where c is a constant. This is a typical behavior of the error of the DE-formula.

It is known that in general the error ΔI_h arising in the numerical integration of an analytic function $f(x)$ can be expressed as [5]

$$\Delta I_h = \frac{1}{2\pi i}\int_C \Phi_h(z) f(z)\,dz, \tag{18}$$

where $\Phi_h(z)$ is called the characteristic function of the error. It depends only on the formula and is independent of the integrand. Specifically the error of the trapezoidal rule with mesh size h applied to the integral

$$I = \int_{-\infty}^{+\infty} g(t)\,dt \tag{19}$$

is given by

$$\Delta I_h = \frac{1}{2\pi i}\int_{\hat{C}} \hat{\Phi}_h(w) g(w)\,dw, \tag{20}$$

where

$$\hat{\Phi}_h(w) = \begin{cases} \dfrac{-2\pi i}{1-\exp(-2\pi i w/h)}, & \text{Im } w > 0, \\ \dfrac{+2\pi i}{1-\exp(+2\pi i w/h)}, & \text{Im } w < 0. \end{cases} \tag{21}$$

$\hat{C}$ consists of two infinite curves, one of which runs to the left above the real axis and the other to the right below the real axis in such a way that there exists no singularity of $g(w)$ between these two curves. Therefore, if we apply the transformation $x = M\phi(t)$ to the integral

$$I = \int_0^\infty f(x)\,dx, \tag{22}$$

and integrate it by the trapezoidal rule, we have from (20)

$$\Delta I_h = \frac{1}{2\pi i}\int_{\hat{C}} \hat{\Phi}_h(w) f(M\phi(w)) M\phi'(w)\,dw \tag{23}$$

$$= \frac{1}{2\pi i}\int_C \Phi_h(z) f(z)\,dz, \quad z = M\phi(w). \tag{24}$$

The relation between the characteristic function $\Phi_h(z)$ in (24) and the function $\hat{\Phi}_h(w)$ in (23) is

$$\Phi_h(z) = \Phi_h(M\phi(w)) = \hat{\Phi}_h(w), \tag{25}$$

and the path C in (24) is the image of $\hat{C}$ in (23) by the mapping $z = M\phi(w)$.

If $|\text{Im } w|$ is not too small, then we have

$$\frac{1}{2\pi}|\hat{\Phi}_h(w)| \approx \exp\left(-\frac{2\pi}{h}|\text{Im } w|\right), \tag{26}$$

and we see that the contour map of the error $|\hat{\Phi}_h(w)|/(2\pi) = 10^{-m}$, $m = 1, 2, \ldots$, consists of lines parallel to the real axis with the equal distance $h \log 10/(2\pi)$.

Figure 3 is a contour map of $|\Phi_h(z)|/(2\pi)$ in the z-plane. This is obtained by actual mapping using a computer of the lines in the w-plane mentioned above onto the z-plane through

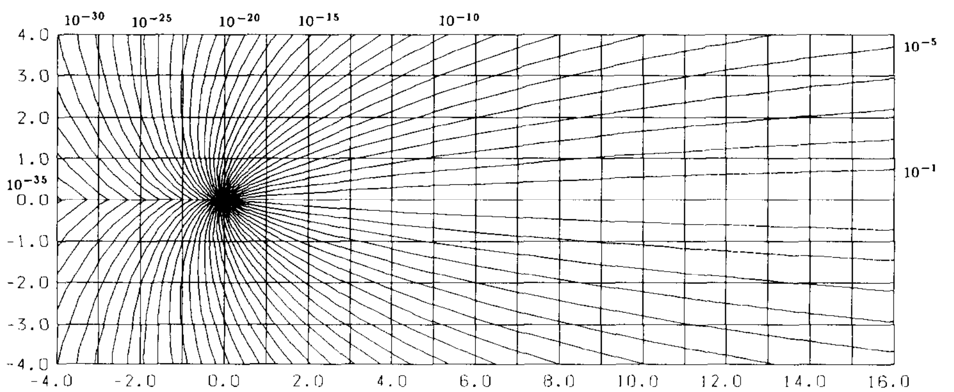

Fig. 3. The contour map of the characteristic function of the error $(2\pi)^{-1}|\Phi_h(z)| = 10^{-m}$, $m = 1, 2, \ldots$, of the formula obtained by $z = M\phi(w) = Mw/\{1-\exp(-6\sinh w)\}$, $M = 64$.

$z = M\phi(w)$. In this figure we see that, since $z = M\phi(w)$ becomes $z \sim Mw$ for large Re w, the contour curves in the map of $|\Phi_h(z)|/(2\pi)$ also approach to lines parallel to the real axis for large Re z, i.e.,

$$\frac{1}{2\pi}|\Phi_h(z)| \approx \exp\left(-\frac{2\pi}{\lambda}|\mathrm{Im}\ z|\right), \quad \text{for large Re } z. \tag{27}$$

The error of the DE-formula is estimated in terms of the error integral (23) and its overall contribution to the error can be divided into the following three parts:

(1) contribution from the part where Re w is negative and large;

(2) contribution from the part where Re w is positive and large;

(3) contribution from the part around the singularities of $f(x)$.

The contributions (1) and (3) are essentially the same as already discussed in the preceding paper [6], i.e., these contributions, as also seen from (21), behave as $\exp(-C/h)$. What should be discussed here is the contribution (2). The reason why the original DE-formula fails to integrate functions which include sin or cos term times slowly decaying function also exists in this point. In the present formula, the characteristic function of the error behaves like (27), and hence, even if $f(x)$ includes the factor $\sin \omega x$ or $\cos \omega x$, $|\Phi_h(z)f(z)|$ decays exponentially as $|\mathrm{Im}\ z|$ becomes large as long as $|\omega| < 2\pi/\lambda$. Therefore we can take the path C of the error integral (24) sufficiently far from the real axis and see that the contribution (2) to the error is small. Consequently we see that the error behaves also as approximately proportional to $\exp(-C/h)$.

There remains one crucial point to be mentioned. Since we assumed that the decay of $f(x)$ is slow for large positive x, we must take a large number of sampling points if there is no additional condition. However, the points of the present formula approach to the zeros of $\sin \omega x$ or $\cos \omega x$ double exponentially for large positive x, so that we need not evaluate $f(x)$ for large x and can truncate the infinite sum (6) at a moderate value of n. In conclusion, the efficiency of the present formula is almost the same as the original DE-formula.

3. Numerical examples

In this section we give some numerical examples of integration using the formula based on the transformation

$$x = M\phi(t), \quad \phi(t) = \frac{t}{1 - \exp(-6 \sinh t)}. \tag{28}$$

We wrote an automatic integrator based on this transformation and compared the results by this integrator with those obtained by other integrators known to be efficient for integrals with sin or cos term. Our integrator chooses automatically an optimal value of M or $h = \pi/M$ corresponding to the error tolerance ϵ given by the user. We computed the following four integrals:

$$I_1 = \int_0^\infty e^{-x} \cos x \, dx = 1, \qquad I_2 = \int_0^\infty \frac{x \sin x}{1 + x^2} \, dx = \frac{\pi}{2e},$$

$$I_3 = \int_0^\infty \frac{\cos x}{1 + x^2} \, dx = \frac{\pi}{2e}, \qquad I_4 = \int_0^\infty \log\frac{x^2 + 4}{x^2 + 1} \cos x \, dx = (e^{-1} - e^{-2})\pi.$$

The result is shown in Table 1. The efficiency of our integrator is compared with an integrator in Hasegawa–Torii [1] and with DQAWF in QUADPACK [3] which is cited also in

Table 1
Comparison of the present integrator based on (28) with other integrators; N is the number of function evaluations

Integral	ϵ = absolute error tolerance $=10^{-6}$						ϵ = absolute error tolerance $=10^{-12}$					
	Present DE		Hasegawa–Torii		QUADPACK		Present DE		Hasegawa–Torii		QUADPACK	
	N	Error	N	Error	N	Error	N	Error	N	Error	N	Error
I_1	22	$1\cdot10^{-8}$	33	$3\cdot10^{-9}$	150	$3\cdot10^{-16}$	54	$4\cdot10^{-14}$	61	$5\cdot10^{-16}$	280	$5\cdot10^{-12}$
I_2	24	$3\cdot10^{-7}$	45	$1\cdot10^{-6}$	385	$3\cdot10^{-9}$	71	$2\cdot10^{-14}$	94	$4\cdot10^{-15}$	700	$8\cdot10^{-13}$
I_3	28	$4\cdot10^{-7}$	57	$1\cdot10^{-8}$	335	$7\cdot10^{-10}$	83	$2\cdot10^{-14}$	93	$1\cdot10^{-13}$	675	$3\cdot10^{-13}$
I_4	29	$1\cdot10^{-7}$	49	$4\cdot10^{-8}$	335	$2\cdot10^{-9}$	84	$1\cdot10^{-13}$	94	$1\cdot10^{-14}$	670	$7\cdot10^{-13}$

[1].

Our integrator is robust against the end point singularity at the origin because it behaves essentially in the same way at the origin as the original DE-formula, as is already mentioned. We computed the following four integrals:

$$I_5=\int_0^\infty \frac{\sin x}{x}\,dx=\tfrac{1}{2}\pi, \qquad I_6=\int_0^\infty \frac{1}{\sqrt{x}}\sin x\,dx=\sqrt{\tfrac{1}{2}\pi},$$

$$I_7=\int_0^\infty \frac{1}{\sqrt{x}}\cos x\,dx=\sqrt{\tfrac{1}{2}\pi}, \qquad I_8=\int_0^\infty \sin x\log x\,dx=-\gamma.$$

The result is given in Table 2. The integrand in I_5 has a removable singularity and it is not difficult to integrate it with any other integrator. The integrand in I_6 decays very slowly at large x. The integrand in I_7 has a singularity at the origin and decays very slowly at large x. The integrand in I_8 has a diverging factor log x and I_8 should be defined as an analytic continuation of

$$\int_0^\infty e^{-zx}\sin x\log x\,dx \tag{29}$$

to $z\to0$. Even if the user is not aware of the existence of this diverging factor our integrator gives the correct result.

In conclusion, the formula presented here is quite efficient for integrals of slowly decaying functions with periodic zeros over the half infinite interval.

Table 2
The result of automatic integration by the integrator based on (28) for integrals of singular or slowly decaying functions; ϵ is the given error tolerance and N is the number of function evaluations

Integral	$\epsilon=10^{-6}$		$\epsilon=10^{-12}$	
	N	Error	N	Error
I_5	30	$6\cdot10^{-9}$	86	$9\cdot10^{-14}$
I_6	28	$4\cdot10^{-9}$	82	$4\cdot10^{-14}$
I_7	35	$3\cdot10^{-8}$	99	$6\cdot10^{-14}$
I_8	29	$3\cdot10^{-7}$	80	$1\cdot10^{-12}$

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