

Numerical Evaluation of Integrals with Infinite Limits and Oscillating Integrands

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The numerical evaluation of slowly convergent integrals with infinite limits and regularly oscillating analytic integrands is discussed. Functions are presented that can be subtracted from the integrands to increase the rate of convergence. One of the integrals used as an example is an often-studied Fourier integral related to the power spectrum of a phase-modulated wave. It is pointed out that, when Fourier integrals whose values are known to be positive, e.g., probability densities, are evaluated by the trapezoidal rule, the values given by the trapezoidal rule are never less than the true values.

I. INTRODUCTION

This paper is in the nature of an addendum to an earlier paper in this journal dealing with the numerical evaluation of definite integrals.¹

Integrals with infinite limits and oscillating integrands often arise in technical problems. In this paper, we assume that the integrand is an analytic function of the variable of integration u (in a suitable region) and tends to oscillate at a regular rate as $u \rightarrow \infty$. The main concern here is how to deal with cases in which the rate of convergence is slow.

A number of ways have been proposed to handle the slow convergence. One is to use integration formulas of Filon's type. In particular, E. O. Tuck² has given a formula of this type suited to an infinite range of integration. Another method is to evaluate the contributions of positive and negative loops of the integrand and apply Euler's summation formula for slowly converging alternating series. Still another is to (i) write the integrand in terms of complex exponentials, (ii) deform the path of integration so that it becomes a path (or portions of paths) of steepest descent in the complex u -plane, and then (iii) integrate along straight-line segments that approximate the path. A closely related procedure is to tilt the path of integration, if possible, so that the integrand will decrease exponentially.

In this paper most of our attention will be devoted to still another method of improving the convergence, namely, that of subtracting from the integrand functions that behave like the leading terms in the asymptotic expansion of the integrand. This method is quite old. It is related to a method used by Kummer to deal with series, and its application to integrals is described by Krylov.³

Sections II through V are concerned with functions useful for subtraction when the limits of integration are 0 and ∞ . Section VI deals with the evaluation of

$$J(b, a) = e^{-b} \int_{-\infty}^{\infty} [\exp(bu^{-1} \sin u) - 1 - bu^{-1} \sin u] e^{iau} du, \quad (1)$$

which serves as a typical example of a slowly converging Fourier integral with limits $\pm \infty$.

The integral (1) has been the subject of several papers because of its relation to the problem of calculating the power spectrum of a phase-modulated wave (see Prabhu and Rowe⁴ and the references they give). In Section VI, results of trial calculations are presented that show that (1) can be efficiently evaluated by the trapezoidal rule after suitable functions have been subtracted from the integrand.

Sections VII and VIII are concerned with the error introduced when a general Fourier integral with limits $\pm \infty$ is evaluated by the trapezoidal rule.

II. PROPERTIES OF FUNCTIONS SUITABLE FOR SUBTRACTION— LIMITS 0 AND ∞

Let the integral to be evaluated be

$$I = \int_0^{\infty} f(u) du,$$

and let the leading term in the asymptotic expansion of $f(u)$ for large u be $u^{-\nu} \exp(iau)$, where a is real and $\nu > 0$. Quite often, in performing numerical integrations, this leading term is subtracted from the integrand only for values of u that exceed some large value U . We have a slightly different procedure in mind here.

Here we want to use the trapezoidal rule methods described in Ref. 1. Since these methods require the integrand to be analytic, we assume that $f(u)$ is analytic in a region containing the positive real axis. Our aim is to subtract an analytic function (which approaches $u^{-\nu} \exp(iau)$ as $u \rightarrow \infty$) from $f(u)$ over the *entire* interval $(0, \infty)$. When this is done, the resulting integral has an integrand analytic over $(0, \infty)$ and can be evaluated by the trapezoidal rule methods described in Ref. 1 (see especially Section IX).

Functions suitable for subtraction when the limits are 0 and ∞ should have the following properties:

- (i) As $u \rightarrow \infty$, they should be asymptotic to $u^{-\nu} \cos au$ or $u^{-\nu} \sin au$ or, more generally, to

$$u^{-\nu} \exp(iau), \quad (2)$$

where $\nu > 0$ and a is real.

- (ii) They should be easy to compute and they should remain finite at $u = 0$.
 (iii) Their integrals between the limits (0, ∞) should be easy to compute.

In some cases, moderately simple functions can be used for subtraction. If the leading term in the asymptotic expansion of the integrand is $(\sin au)/u$, then we can subtract and add the integral

$$\int_0^{\infty} u^{-1} \sin au \, du = \begin{cases} \pi/2, & a > 0 \\ -\pi/2, & a < 0. \end{cases} \quad (3)$$

Similarly, for $(\cos au)/u$ we can use

$$\int_0^{\infty} u^{-1} [\cos au - \exp(-au)] du = 0, \quad (4)$$

and, for $(\cos au)/u^2$,

$$\int_0^{\infty} (\cos au) du / (1 + u^2) = \frac{1}{2} \pi \exp(-|a|). \quad (5)$$

The last integral (5) has the disadvantage that its integrand has the asymptotic expansion

$$\frac{\cos au}{u^2} - \frac{\cos au}{u^4} + \dots, \quad (6)$$

and if we desire to subtract terms of both $O(u^{-2})$ and $O(u^{-4})$ from the original integrand, the term $-(\cos au)/u^4$ in (6) has to be taken into account. In the applications we have in mind, the $\exp(-au)$ in (4) decreases so rapidly that it does not have to be taken into account in the way that $-(\cos au)/u^4$ does.

III. GENERAL FUNCTIONS FOR SUBTRACTION—LIMITS 0 AND ∞

Here we present a set of functions that meets the "ease of computation" requirements (ii) and (iii) reasonably well. It is quite likely that there are better sets, but this one is the best I have been able to find. There are two formulas according to whether ν is an integer or not.

The functions are the integrands in

$$\int_0^{\infty} u^{-n-\epsilon} (e^{-\alpha u} - e^{-\beta u})^n du = \frac{\Gamma(1-\epsilon)}{(\epsilon)_n} \sum_{k=0}^n (-)^{n-k} \binom{n}{k} \times [(n-k)\alpha + k\beta]^{n+\epsilon-1}, \quad (7)$$

$$\int_0^{\infty} \left(\frac{e^{-\alpha u} - e^{-\beta u}}{u} \right)^n du = \frac{1}{(n-1)!} \sum_{k=0}^n (-)^{n-k} \binom{n}{k} \times [(n-k)\alpha + k\beta]^{n-1} \ln [(n-k)\alpha + k\beta], \quad (8)$$

where n is a positive integer and n, α, β , and ϵ are such that the integrals converge. In (7), ϵ is not an integer, and $(\epsilon)_0 = 1$, $(\epsilon)_n = \epsilon(\epsilon+1)\cdots(\epsilon+n-1)$. In using (7) and (8), we set $\alpha = -ia/n$, $\beta = |a|/n$. In (7), n and ϵ are chosen so that $\epsilon < -1$ and $n + \epsilon$ is equal to the exponent ν in (2). The choice $\epsilon < -1$ is made to make the integrand and its derivative in (7) approach 0 as $u \rightarrow 0$. This tends to reduce the error in the numerical integration. Since a can be either positive or negative in $\alpha = -ia/n$ and $\beta = |a|/n$, we take

$$-\pi/2 \leq \arg [(n-k)\alpha + k\beta] \leq \pi/2$$

when calculating the logarithm and the $(n + \epsilon - 1)$ th power of $[(n-k)\alpha + k\beta]$.

Equation (8) is obtained by letting $\epsilon \rightarrow 0$ in (7), and (7) is based upon (page 243 of Ref. 5)

$$\Gamma(1-n-\epsilon) = \int_0^{\infty} \frac{dt}{t^{n+\epsilon}} \left\{ e^{-t} - \sum_{l=0}^{n-1} \frac{(-t)^l}{l!} \right\}, \quad (9)$$

where, in contrast to (7), ϵ is restricted to $0 < \epsilon < 1$ to secure convergence. To obtain (7), expand $[\exp(-\alpha u) - \exp(-\beta u)]^n$ by the binomial theorem. Then to each term $\exp[-(n-k)\alpha u - k\beta u]$, add and subtract the series

$$- \sum_{l=0}^{n-1} (-u)^l [(n-k)\alpha + k\beta]^l / l!$$

Equation (7) then follows from (9) with $t = [(n-k)\alpha + k\beta]u$ and the relation

$$\sum_{k=0}^n (-)^k \binom{n}{k} [(n-k)\alpha + k\beta]^l = 0, \quad (10)$$

where $l = 0, 1, \dots, n-1$. Equation (10) expresses the fact that u^n is the lowest power of u in the power series for $[\exp(-\alpha u) - \exp(-\beta u)]^n$. After (7) has been established for $0 < \epsilon < 1$, it can be extended by analytic continuation to the values of ϵ needed in the application of (7).

Other choices of α and β besides $-ia/n$ and $|a|/n$ can be made in (7) and (8). In some cases, it may be better to take $\alpha = -ia/n$ and

$\beta = \alpha + b$, where b is a positive constant at our disposal. For this choice of α and β , $[\exp(-\alpha u) - \exp(-\beta u)]^n$ becomes $\exp(iau) \times [1 - \exp(-bu)]^n$ and $(n-k)\alpha + k\beta$ becomes $kb - ia$. By using these values in (7), equating imaginary parts, and letting $\epsilon \rightarrow 1$, we can obtain

$$\int_0^\infty u^{-n-1}(1 - e^{-bu})^n \sin au \, du = \text{Im} \frac{1}{n!} \sum_{k=0}^n (-)^{n-k} \binom{n}{k} (kb + ia)^n \ln(kb + ia).$$

Here the integrand tends to $(\sin au)/u^{n+1}$ as $u \rightarrow \infty$.

IV. EXAMPLE ILLUSTRATING APPLICATION OF EQ. (8)

Consider the integral

$$I = \int_0^\infty (1 + u^2)^{-\frac{1}{2}} e^{iu} \, du, \quad (11)$$

which is equal to $K_0(1) + i\pi[I_0(1) - L_0(1)]/2$, where K_0 and I_0 are Bessel functions and L_0 is a Struve function (page 498 of Ref. 6). As $u \rightarrow \infty$, the integrand approaches

$$u^{-1}e^{iu} - \frac{1}{2}u^{-3}e^{iu} + \dots$$

Therefore, if we desire convergence like that of $u^{-5}e^{iu}$, we apply (8) twice. First with $n = 1$, $\alpha = -i$, $\beta = 1$, and then with $n = 3$, $\alpha = -i/3$, $\beta = \frac{1}{3}$:

$$I = \int_0^\infty du \left[(1 + u^2)^{-\frac{1}{2}} e^{iu} - \left(\frac{e^{iu} - e^{-u}}{u} \right) + \frac{1}{2} \left(\frac{e^{iu/3} - e^{-u/3}}{u} \right)^3 \right] + \frac{1}{0!} [-\ln(-i) + \ln(1)] - \frac{1}{2} \frac{1}{2!} \sum_{k=0}^3 \binom{3}{k} (-)^{3-k} [(3-k)(-i/3) + k/3]^2 \times \ln[(3-k)(-i/3) + k/3]. \quad (12)$$

The second line reduces to $i\pi/2$ [which, incidentally, gives the combination of (3) and (4)]. Although the last sum appears complicated, it can be readily evaluated by a digital computer when the program is written using complex variables.

The integrand in (12) now decreases as $u^{-5}e^{iu}$ when u is large, and the integral can be evaluated by any suitable method of numerical integration. Some computations were made using the trapezoidal rule as described in Section IX of Ref. 1. In this method, the variable of integration is changed from u to x , where $u = a \ln[1 + \exp(x/a)]$, and the integral in x is evaluated by the trapezoidal rule. A computation using 52 points with $h = \Delta x = 4.0$ and $a = 6$ gave $I = 0.42102 \dots + i0.87308 \dots$, which agrees with tabulated values.

This example brings to mind the question, when does one cease subtracting terms from the integrand and start integrating? That is, what is the trade-off between computing trapezoidal sums and those sums in (7) and (8)? There seems to be no well-defined answer, but experience indicates that there is usually no need to make the integrand decrease faster than the inverse fifth or sixth power of the variable of integration.

Incidentally, the integral for I is quite readily evaluated by tilting the path of integration. Arbitrarily choosing a 45-degree tilt and setting $u = (1 + i)t$ carries (11) into

$$I = \int_0^{\infty} e^{-t} f(t) dt, \\ f(t) = (1 + i)(1 + 2it^2)^{-1/2} e^{it}. \quad (13)$$

The contribution of the 45-degree arc at $|u| = \infty$ is zero by Jordan's lemma (page 115 of Ref. 5). The integral is now in the form discussed in Section VI of Ref. 1, and can be efficiently evaluated by the trapezoidal rule after the change of variable $t = e^v$, $v = x - e^{-x}$. Computations made with this example suggest that when "tilting" can be used, it is preferable to "subtraction." However, tilting cannot always be used, an example being the integral $J(b, a)$ defined by (1).

V. EXAMPLE ILLUSTRATING THE USE OF EQ. (7)

Consider the integral

$$I = \int_0^{\infty} (1 + u^2)^{-5/6} e^{iu} du, \quad (14)$$

the real part of which is related to the Bessel function $K_{1/3}(1)$. When $u \rightarrow \infty$, the integrand becomes

$$u^{-5/3} e^{iu} + O(u^{-11/3}).$$

Therefore, to secure convergence of $O(u^{-11/3})$, we apply (7) once with $n + \epsilon = 5/3$. Since n must be a positive integer, possible choices of ϵ are $2/3, -1/3, -4/3, \dots$. We also want $\epsilon < -1$. We arbitrarily choose $\epsilon = -4/3$ (and therefore $n = 3$) to make the integrand of (7) tend to 0 as $u^{4/3}$ when $u \rightarrow 0$. Because $n = 3$ we take $\alpha = -i/3$ and $\beta = 1/3$. Then

$$I = \int_0^{\infty} du [(1 + u^2)^{-5/6} e^{iu} - u^{-5/3} (e^{iu/3} - e^{-u/3})^3] \\ + \frac{\Gamma(7/3)}{(-4/3)(-1/3)(2/3)} \sum_{k=0}^3 (-)^{3-k} \binom{3}{k} \\ \times [(3 - k)(-i/3) + (k/3)]^{2/3}. \quad (15)$$

This integral can be evaluated by the trapezoidal rule in much the same way as was the integral in (12).

VI. NUMERICAL EVALUATION OF THE INTEGRAL $J(b,a)$

To simplify the discussion of $J(b, a)$ defined by the integral (1), we assume that b is positive. The parameter a is real and $J(b, a)$ is an even function of a .

The integrand in $J(b, a)$ can be expanded as $\exp(iau)$ times

$$\sum_{n=2}^{\infty} (bu^{-1} \sin u)^n/n!,$$

and the term for $n = 2$ shows that the integral converges slowly. Inspection shows that the rate of convergence can be increased by writing $J(b, a)$ as an integral from 0 to ∞ and subtracting terms of the form $u^{-n} \exp(iau)$ as described in Sections III and IV. However, it is more convenient to subtract terms of the form $(u^{-1} \sin u)^n$ and use the known values of

$$B_n = \int_{-\infty}^{\infty} (bu^{-1} \sin u)^n \cos au \, du/n!, \quad (16)$$

where $n \geq 1$ is an integer and B_n is an even function of a .

When $n = 1$, B_1 is equal to $b\pi$ for $|a| < 1$, to $b\pi/2$ for $|a| = 1$, and to 0 for $|a| > 1$. When $n \geq 2$, B_n is a continuous function of a which is 0 when $|a| \geq n$. When $n \geq 2$ and $|a| \leq n$,

$$B_n = \frac{2\pi(b/2)^n}{n!(n-1)!} \sum_{m=0}^M (-)^m \binom{n}{m} (n \pm a - 2m)^{n-1}, \quad (17)$$

where M is the integer part of $(n \pm a)/2$. The choice of the sign in \pm is arbitrary, but it must be the same in M and in (17). The minus sign is the more convenient choice when $a > 0$.

When we desire convergence at the rate of, say, $1/u^6$, we subtract and add $e^{-b}(B_2 + B_3 + B_4 + B_5)$:

$$J(b, a) = e^{-b} \int_{-\infty}^{\infty} \left[\exp(bu^{-1} \sin u) - 1 - \sum_{n=1}^5 (bu^{-1} \sin u)^n/n! \right] e^{iau} du + e^{-b}(B_2 + B_3 + B_4 + B_5). \quad (18)$$

Incidentally, $J(b, a)$ is equal to e^{-b} times the infinite sum $B_2 + B_3 + \dots$, a result useful for computation when b is small.

The integrand in (18) is an analytic function of u , and the results of Ref. 1 suggest direct numerical integration by the trapezoidal rule. Several trial computations were made to obtain an idea of the performance of this method of integration. In the actual work, the integral

Table I — Values of $J(b,a)$ obtained by the trapezoidal rule

b	a	h	N	u_{\max}	$J(b, a)$
1	1	0.7	12	7.7	0.413 5433
1	4	0.4	20	7.6	0.000 0428
4	1	0.5	36	17.5	1.341 1671
4	4	0.4	45	17.6	0.011 6253
16	1	0.3	39	11.4	0.997 3179
16	10	0.225	52	11.5	0.000 2046
32	1	0.25	19	4.5	0.736 6452
32	10	0.175	26	4.4	0.007 6251

was rewritten as an integral from 0 to ∞ , and $\exp(iau)$ was replaced by $\cos au$. Typical results are shown in Table I. Here N is the number of terms in the trapezoidal sum, and h is the spacing between successive values of u . The trapezoidal sum was truncated at $u = u_{\max} = (N - 1)h$. I believe the values shown for $J(b, a)$ are accurate to the number of places shown. A short table of $J(b, a)$ for $a \leq 1.25$ is given in Ref. 7, where $J(b, a)e^b$ is referred to as "Lewin's integral." When b is large, the work of Prabhu and Rowe⁴ gives tight bounds on $J(b, a)$ for all values of a .

The truncation value u_{\max} was chosen to be the value of u beyond which the absolute value of the integrand remains less than 10^{-8} . This makes the truncation error less than $10^{-8}u_{\max}/5$. It can be shown that u_{\max} has a maximum value of about 18 near $b = 6$.

The error E in the computed value of $J(b, a)$ resulting from the finite size of the spacing h , i.e., the "trapezoidal error," is of the order of $J(b, 2\pi h^{-1} - a)$ when h is small. This follows from Section VII below. The trapezoidal errors observed in the construction of Table I agree well with the values of $J(b, 2\pi h^{-1} - a)$ estimated from bounds for $J(b, a)$ given by Prabhu and Rowe.⁴ E decreases rapidly as h decreases through the values shown in Table I.

VII. TRAPEZOIDAL ERROR FOR FOURIER INTEGRALS

Let the Fourier integral and the associated trapezoidal error be, respectively,

$$I(a) = \int_{-\infty}^{\infty} F(u)e^{iau} du, \quad (19)$$

$$E = h \sum_{n=-\infty}^{\infty} F(nh) \exp(ianh) - I(a). \quad (20)$$

As in Ref. 1, Poisson's summation formula gives

$$E = \left(\sum_{k=-\infty}^{-1} + \sum_{k=1}^{\infty} \right) I(2\pi kh^{-1} + a). \quad (21)$$

When $F(u)$ is an even function of u , $I(-a)$ is equal to $I(a)$, and (21) gives

$$E = \sum_{k=1}^{\infty} [I(2\pi kh^{-1} - a) + I(2\pi kh^{-1} + a)]. \quad (22)$$

It is interesting to note that, if $I(a)$ is known to be real and nonnegative for all real values of a , then E is nonnegative and the values of $I(a)$ obtained by evaluating (19) by the trapezoidal rule are always greater than or equal to the true value of $I(a)$, truncation errors aside. This fact is of use in dealing with power spectra and probability densities.

Now let $F(u)$ be analytic in a strip in the u -plane containing the real u -axis. When $F(u)$ is even and analytic, usually only the $k = 1$ term in (22) is important if h is small. In addition, if $a > 0$, E and $I(2\pi h^{-1} - a)$ are usually of the same order of magnitude.

VIII. DISPLACING THE PATH OF INTEGRATION OF A FOURIER INTEGRAL

In some cases, the numerical evaluation of the Fourier integral $I(a)$ defined by (19) can be facilitated by shifting the path of integration from the real u -axis to a parallel path that passes through $u = ic$, where c is some suitably chosen real constant. Changing the variable of integration in the integral (19) for $I(a)$ from u to x , where $u = x + ic$, and applying the trapezoidal rule to the integral in x gives the trapezoidal error

$$E' = h \sum_{n=-\infty}^{\infty} F(nh + ic)e^{ianh-ac} - I(a),$$

which, by Poisson's summation formula, goes into

$$E' = \left(\sum_{k=-\infty}^{-1} + \sum_{k=1}^{\infty} \right) I(2\pi kh^{-1} + a)e^{2\pi kc/h}. \quad (23)$$

When $I(a)$ is known to be real and nonnegative for all real values of a , then E' is nonnegative just as E is in (21), and the trapezoidal values of $I(a)$ obtained from the displaced path are greater than or possibly equal to the true value of $I(a)$, just as before.

The integral in the expression (18) for $J(b, a)$ is of the Fourier type (19), and some calculations were made to test the benefit obtained by shifting the path of integration. Along the path $u = x + ic$, the real part of the integrand is an even function of x , and the integral in (18) can be rewritten as an integral from $x = 0$ to ∞ of twice the real part. For $b = 32$ and $a = 10$, the value of c was chosen to be 0.87. This corresponds to the saddle point $u_0 = i0.87$ of $\exp(bu^{-1} \sin u + iau)$. A trapezoidal rule evaluation with $h = 0.3$ along the line $u = x + i0.87$ gave $J(b, a)$ to the accuracy shown in Table I. The number of terms

required was $N = 16$ compared with $N = 26$ when the integration was taken along the real u -axis (with $h = 0.175$).

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