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Note

More on the Calculation of Oscillatory Integrals

The numerical evaluation of integrals of the type

$$\int_0^\infty g(t) \cos \zeta t \, dt \tag{1}$$

(with emphasis on large values of ζ) was the subject of a recent paper by Boris and Oran [1]. In this note, we shall show that the application of the Poisson summation formula leads to an even simpler algorithm for the numerical computation of such integrals, and, in addition, provides a priori estimates of the error which would otherwise be unavailable.

The form of Poisson's formula which is applicable to integrals of type (1) is [2]

$$\int_0^\infty f(t) \, dt = h[\tfrac{1}{2} f(0) + f(h) + f(2h) + \cdots +] - 2 \sum_{k=1}^{\infty} F\left(\frac{2k\pi}{h}\right), \tag{2}$$

where h is an arbitrary positive quantity, and $F(y)$ is the Fourier cosine transform of $f(t)$:

$$F(y) = \int_0^\infty f(t) \cos yt \, dt. \tag{3}$$

(For additional applications, see [3, 5, 6].) In particular, if $f(t)$ is an even function which tends exponentially to zero as $t \to \infty$, the transform function $F(y)$ also vanishes exponentially as $y \to \infty$ (i.e., as $h \to 0$). In this instance, the error in approximating the integral in Eq. (2) by the first infinite sum of the R.H.S. can be determined essentially from the magnitude of $F(2\pi/h)$, and this, because of the property of $F(y)$ just noted, can be made arbitrarily small by taking h sufficiently small. If, in addition, the asymptotic behavior of $F(y)$ for large y is known, an a priori estimate of the value of h necessary to obtain a prescribed accuracy is available.

For integrals of type (1), $f(t)$ in Eq. (3) is replaced by

$$g(t) \cos \zeta t,$$

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and Eq. (2) modified to read

$$\int_0^\infty g(t)\cos\zeta t\,dt = h[\tfrac{1}{2}g(0) + g(h)\cos(\zeta h) + g(2h)\cos(2\zeta h) + \cdots +]$$
$$- \sum_{k=1}^{\infty}\left[G\left(\frac{2k\pi}{h}+\zeta\right)+G\left(\frac{2k\pi}{h}-\zeta\right)\right], \tag{4}$$

where $G(y)$ is now the Fourier transform of $g(t)$ as defined by analogy to Eq. (3).

Now when h is small and $2\pi/h \gg \zeta$, the magnitude of $G((2\pi/h)-\zeta)$ will dominate that of $G((2\pi/h)+\zeta)$, so that the magnitude of the error term which, as noted above, is essentially that of the first term of the series, can be estimated by that of

$$G((2\pi/h)-\zeta). \tag{5}$$

The two examples in [1] can be used to illustrate this. In the first of these, we have

$$g(t) = (\cosh xt)^{-1} \tag{6}$$

and

$$G(y) = \pi/2x\cosh(\pi y/2x). \tag{7}$$

Hence the error estimate is

$$E(h) \cong \pi/2x\cosh(\pi/2x)((2\pi/h)-\zeta) < (\pi/x)\,e^{\pi\zeta/2x}e^{-\pi^2/xh}, \tag{8}$$

which, with $x=2$ and $\zeta=4$, becomes

$$E(h) \cong 36.35\,e^{-\pi^2/2h}. \tag{9}$$

A convenient choise of h is π/m, where m is an integer; this causes the integrand to be evaluated at integral subdivisions of π. In particular, if m is even, two of the evaluation points in each cycle will occur when $\zeta t = \pi/2 + k\pi$, $3\pi/2 + k\pi$,..., at which points the integrand will be zero. The value $h = \pi/16$, for example, leads to the error estimate

$$E(\pi/16) \cong 4.42 \times 10^{-10}, \tag{10}$$

which is in agreement with the results of [1, Table I, $N=4$]. (Note that, although the value $N=4$ would normally imply 8 evaluations per cycle, the number of actual evaluations is only 6, for the reason given above.)

In the second example,

$$g(t) = e^{-x\cosh t}, \qquad G(y) = \int_0^\infty e^{-x\cosh t}\cos yt\,dt = K_{iy}(x), \tag{11}$$

which, for large y has the asymptotic behavior

$$G(y) \cong e^{-(\pi/2)y}, \tag{12}$$

so that an estimate of the error is

$$E(h) \cong e^{-(\pi/2)((2\pi/h)-\zeta)}. \tag{13}$$

(For more precise estimates, see [4].) Since, in this example, ζ is large, h must be chosen sufficiently small so that $2\pi/h \gg \zeta$. Also, since the magnitude of the integral will be correspondingly small, the number of decimal places in the error term will not be a true indication of the number of correct significant figures obtained. In such cases, it is preferable, therefore, to have an estimate of the relative error

$$E_r(h) = e^{(\pi/2)y} E(h) \cong e^{-\pi((\pi/h)-\zeta)}. \tag{14}$$

With $\zeta = 39$, the choice $h = \pi/78$ leads to a relative error estimate of 6×10^{-54}, which far exceeds any accuracy which would normally be needed (or even attainable), but it is indicative of the high degree of accuracy that can be obtained for such integrals.

In the example, the magnitude of the integral itself, as estimated by the asymptotic behavior given by Eq. (12), differs from that of the largest ordinate (at $t = 0$) by approximately 10^{-8}. This means that there will be a loss of at least the first 8 figures due to cancellation of positive and negative quantities in the summation. This cancellation must be compensated for by a sufficiently high degree of precision in the calculations. The following computations were carried out for the second example on

TABLE I

Evaluation of $K_{i\zeta}(x)$ by Numerical Integration; $x = 40$, $\zeta = 39$

t	$e^{-x\cosh t} \cos \zeta t \times 10^{18}$	
($\frac{1}{2}$) 0	2.12417 71276 458	
$\pi/39$		−3.73102 74327 642
$2\pi 39$	2.52514 00847 368	
$3\pi/39$		−1.31368 45258 740
$4\pi/39$	0.52312 17291 798	
$5\pi/39$		−0.15849 81755 149
$6\pi/39$	0.03625 67429 034	
$7\pi/39$		−0.00620 20756 051
$8\pi/39$	0.00078 43147 193	
$9\pi/39$		−0.00007 23466 183
$10\pi/39$	0.00000 47929 242	
$11\pi/39$		−0.00000 02240 701
$12\pi/39$	0.00000 00072 466	
$13\pi/39$		−0.00000 00001 586
$14\pi/39$	0.00000 00000 023	
Sum	5.20948 47993 583	−5.20948 47806 053

Note. $K_{39i}(40) \cong (\pi/78) \times (1.87530 \times 10^{-26}) = 7.5531 \times 10^{-28}$.

the Lawrence Livermore Laboratory CDC-7600 computer, using both 14 and 26 digit arithmetic. With 14 digits, and knowing that the terminal figures in the intermediate calculations are subject to round off and/or truncation, the final value should be correct to at least 5 figures. This is borne out by the second set of results, where 17 correct figures remain after cancellation. (There would actually be over 40 correct figures, if a sufficient number of digits were available in the arithmetic package.) Numerical details are given in Table I for the 14 digit arithmetic. The final results for both sets are, with $x = 40$, $\zeta = 39$,

$$K_{i\zeta}(x) \cong 7.5531 \times 10^{-28} \qquad \text{(14 digits)},$$

$$K_{i\zeta}(x) \cong 7.553\,05218\,79261 \times 10^{-28} \qquad \text{(26 digits)}.$$

(Note that, in this example, it is only necessary to evaluate the integrand at two points/cycle, and that these occur when $t = 0$, $k\pi/39$, $k = 1, 2, \ldots$, where the value of the cosine is either $+1$ (k even) or -1 (k odd).)

The above results may be compared with the value

$$K_{i\zeta}(x) \cong 7.553054 \times 10^{-28}$$

obtained in [1] with both two and four points/cycle. (The random behavior of the terminal digits in [1, Table II, column 4] leads one to suspect that all of them are unreliable due to round off or truncation, since, as noted above, the integration interval ($\pi/78$) assures at least 17 correct figures in the final answer, provided the arithmetic package which is used contains a sufficient number of working digits.)

References

1. J. P. Boris and E. S. Oran, *J. Comput. Phys.* **17** (1975), 425.
2. W. Magnus and F. Oberhettinger, " Formeln und Sätze für die Speziellen Funktionen der Mathematische Physik," Springer–Verlag, Berlin, 1948.
3. H. E. Fettis, *Math. Comput.* **9** (1955), 85.
4. A. Erdelyi *et al.*, "Higher Transcendental Functions," Vol. 2, p. 87–88, Art. 7.13.2 (18)–(20), McGraw-Hill, New York, 1954.
5. Y. L. Luke, "The Special Functions and Their Approximations," Vol. 2, pp. 214–226, Academic Press, New York/London, 1969.
6. Y. L. Luke, "Mathematical Functions and Their Approximations," pp 134–137, 395–399, Academic Press, New York/London, 1975.

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