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TECHNICAL NOTES AND SHORT PAPERS

A Method for the Numerical Evaluation of Certain Infinite Integrals

The solution of many physical problems often necessitates the numerical evaluation of infinite real integrals, a common example being that of solutions obtained with the aid of integral transforms. The evaluation of such integrals is often a laborious task, particularly if the integrand is oscillatory, so that it is usual to resort to special methods which give information for certain ranges of values of the variables; methods of this type are those involving asymptotic expansions or the related techniques of steepest descent and of stationary phase. The purpose of the present note is to outline a method in which the value of such integrals is expressed in terms of a convergent series obtained by a modification of the corresponding asymptotic expansion. The development is given below for a special case only, namely one which might arise in conjunction with the use of sine transforms; it will be clear however that these results can be readily generalized to other types of integrals which are usually reduced to an asymptotic representation. Examples may be found in Erdélyi [1]. The method is thus valid whether the integrand is oscillatory or not; in fact, though the special integrand considered in detail below does oscillate, inspection of the convergence proofs shows that this fact is of little importance to the developments presented. A method which holds in the case of oscillatory integrands has been described by I. M. Longman [2].

Basic expansions. Consider a convergent integral $I(a)$ of the form

$$(1) \qquad I(a) = \int_a^\infty f(x) \sin x dx; \qquad f(x) \to 0 \text{ steadily as } x \to \infty.$$

By $f(x) \to 0$ steadily, we mean that $f(x_1) \geq f(x_2) > 0$ if $x_1 < x_2$ and $\lim f(x) = 0$; see Whittaker and Watson [3]. N successive integrations by parts may be shown to give the following result

$$(2) \quad I(a) = \sum_{i=0}^{N} f^{(i)}(a) \cos [a + i(\pi/2)] + \int_a^\infty f^{(N)}(x) \sin [x + N(\pi/2)] dx$$

where $f^{(i)} = (d^i f/dx^i)$, provided that $f(x)$ is differentiable the required number of times, and that

$$(2a) \qquad f^{(i)}(x) \to 0 \text{ steadily as } x \to \infty; \qquad i = 0, 1, 2, \cdots.$$

The term in equation (2) containing the summation usually represents an asymptotic representation of I for large values of a, and the infinite series obtained as N is increased indefinitely in general does not converge. A convergent expansion for $I(a)$ may now be derived in the following manner. Integration by parts gives

$$(3a) \qquad I(a) = \int_a^{a_1} f(x) \sin x dx + f(a_1) \cos a_1 + \int_{a_1}^{\infty} f^{(1)}(x) \cos x dx$$

and further

$$(3b) \qquad I(a) = \int_a^{a_1} f(x) \sin x dx + \int_{a_1}^{a_2} f^{(1)}(x) \cos x dx + f(a_1) \cos a_1 - f^{(1)}(a_2) \sin a_2 - \int_{a_2}^{\infty} f^{(2)}(x) \sin x dx.$$

Repetition of this process finally gives

$$(4) \qquad I(a) = \sum_{i=0}^{\infty} f^{(i)}(a_{i+1}) \cos [a_{i+1} + i(\pi/2)] + \sum_{i=0}^{\infty} \int_{a_i}^{a_{i+1}} f^{(i)}(x) \sin [x + i(\pi/2)] dx$$

where one may set

$$(4a) \qquad a_{i+1} \geq a_i; \qquad a_0 = a.$$

It will now be shown that the quantities a_i may be chosen in such a manner that the two series on the right-hand side of equation (4) converge.

Convergence of series expansion. The first series on the right-hand side of equation (4) will certainly converge if the a_i's are chosen so that the series

$$(5) \qquad S_1 = \sum_{i=0}^{\infty} f^{(i)}(a_{i+1})$$

converges; and this series will converge (absolutely) if a positive number ρ independent of i exists such that

$$(5a) \qquad 1 > \rho > \left| f^{(i)}(a_{i+1}) / f^{(i-1)}(a_i) \right|$$

for all $i \geq 1$. It will now be shown that such a choice of a_i's is always possible. (The author is indebted to Dr. C. C. Chao for his valuable suggestions concerning this proof.)

Choose the quantity $a_i \geq a_0$ arbitrarily; then the value of $f^{(0)}(a_1)$ is known and a_2 must be selected so that

$$(5b) \qquad \left| f^{(1)}(a_2) \right| < \rho \left| f^{(0)}(a_1) \right|$$

as may always be done because of relation (2a). Now however the value of $f^{(1)}(a_2)$ is known, and so a_3 can be chosen by a similar procedure. Repetition of this process yields values of all a_i's in such a manner that relation (5a) is satisfied for all $i \geq 1$ and therefore series S_1 converges absolutely. It should be noted that the choice of a_i's is not unique, and that in fact if such a choice has been made ($a_i = a_i'$, say) then the values $a_i = a_i''$ will also insure convergence of S_1 provided only that

$$(6) \qquad a_i'' \geq a_i'$$

in view of the steadiness requirement of equation (2a).

It will now be shown that the a_i's may be taken in conformity with requirement (6) and, in addition, so that the second series of equation (4), namely

$$(7)\qquad S_2 = \sum_{i=0}^{\infty} I_i; \qquad I_i = \int_{a_i}^{a_{i+1}} f^{(i)}(x) \sin [x + i(\pi/2)] dx$$

also converges. Note first that it follows from equation (2a) that, for any i, a number A_i exists such that

$$(7a)\qquad |f^{(i-1)}(x_i)| < |f^{(i-1)}(x)| \qquad \text{for all } x_1 > x > A_i.$$

Let now the quantities a_i be selected (consistently with inequality (6)), so that

$$(7b)\qquad a_i \geqslant A_i.$$

Because of equation (4a) then the relation

$$(7c)\qquad |f^{(i-1)}(a_{i+1})/f^{(i-1)}(a_i)| < 1$$

holds for all i.

Consider now the integrals I_i; because of the steadiness requirement in equation (2a) the quantity $f^{(i)}(x)$ does not change sign within $a_i \leq x \leq a_{i+1}$ and

$$(8a)\qquad |I_i| < \left| \int_{a_i}^{a_{i+1}} f^{(i)}(x) dx \right| = |f^{(i-1)}(a_{i+1}) - f^{(i-1)}(a_i)| =$$

$$|f^{(i-1)}(a_i)| \, 1 - [f^{(i-1)}(a_i + 1)/f^{(i-1)}(a_i)] \, | < 2 \, |f^{(i-1)}(a_i)| \, ; \qquad i \neq 0$$

in view of relation (7c). Series S_2 (with the possible omission of the first term) is then term-by-term less than the series

$$(8b)\qquad 2 \sum_{i=1}^{\infty} |f^{(i-1)}(a_i)| = 2 \sum_{i=0}^{\infty} |f^{(i)}(a_{i+1})|$$

which has been shown to converge. Hence S_2 also converges.

Example. As an illustration of the procedure indicated above, the special case of $f(x) = x^{-k}$ will be considered; thus

$$(9)\qquad I(a) = \int_a^{\infty} x^{-k} \sin x dx; \qquad k > 0.$$

Here one may take (as will be shown)

$$(10)\qquad a_i = a + i\alpha$$

where α is a constant; equation (4) then reduces to

$$(10a)\qquad I(a) = S_1(a) + S_2(a)$$

where

$$S_1(a) = \sum_{i=1}^{\infty} \frac{(1)(k)(k+1) \cdots (k+i-2)}{(a + i\alpha)^{(k+i-1)}} \sin [i(\pi/2 - \alpha) - a]$$

(10b)

$$S_2(a) = \sum_{i=1}^{\infty} (1)(k)(k+1) \cdots (k+i-2) \int_{a+(i-1)\alpha}^{a+i\alpha} x^{-(k+i-1)} \cos [i(\pi/2) - x] dx.$$

Series S_1 converges if

$$(10c)\quad 1 > \lim_{i\to\infty}\left\{\frac{(k+i-1)(a+i\alpha)^{(k+i-1)}}{[a+(i+1)\alpha]^{(k+i)}}\right\}$$

$$= \lim_{i\to\infty}\left(\frac{k+i-1}{a+i\alpha}\right)\lim_{i\to\infty}\left(\frac{a+i\alpha}{a+(i+1)\alpha}\right)^k\lim_{i\to\infty}\left(\frac{a+i\alpha}{a+(i+1)\alpha}\right)^i$$

$$= (1/\alpha)\lim_{i\to\infty}\left(1-\frac{1}{1+(a/\alpha)+i}\right)^i = 1/(\alpha e)$$

or in other words if

$$(10d)\qquad \alpha > (1/e).$$

Series S_2 may now be considered by expanding the integrals it contains in a manner entirely analogous to that of equations (8a) and (8b), and it can thus be easily shown that this series also converges if α is chosen as specified in equation (10d); the latter condition then represents in the present case the only requirement for convergence of expansion (10a).

An advantageous choice of α, consistent with requirement (10d), is $\alpha = \pi/2$, since in this case the sine-term in S_1 is constant; in particular, if $a = 0$ (or $a = n\pi$), note that $S_1 = 0$. No choice of α is of course possible which will make $S_2 = 0$, so that numerical evaluations of integrals are still necessary. Series S_2 converges quite rapidly, however; as an example consider in fact the case of $a = 0$, $k = 1$ and $\alpha = \pi/2$ for which the value of the integral in question is well known. The result may be written as

$$(11)\quad (2/\pi)\int_0^\infty (1/x)\sin x dx = 1 = (2/\pi)\sum_{i=1}^\infty (i-1)!\int_{(i-1)\pi/2}^{i\pi/2} x^{-i} \cos[i(\pi/2)-x]dx.$$

The integrals in this summation were evaluated by Simpson's rule with the relatively coarse interval of $(\pi/8)$. The value of the summation itself may be expressed as the limit of the sequence of the partial sums S_i of the first i terms of the series; the first few terms of this sequence were found to be as follows (to four significant figures):

$$(11a)\quad S_1 = .8727;\quad S_2 = .9762;\quad S_3 = .9951;\quad S_4 = .9988;\quad S_5 = .9996$$

and may therefore be said to converge fairly rapidly. Almost the same results were obtained when the coarser interval of $(\pi/4)$ was used in Simpson's rule.

Bruno A. Boley

Columbia University
New York, New York

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