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

$$ I(a) = \int_{0}^{\infty} f(x) \sin x \, dx; \quad f(x) \to 0 \text{ steadily as } x \to \infty. $$

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

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

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

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

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

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

and further

$$I(a) = \int_a^{a_1} f(x) \sin x \, dx + \int_{a_1}^{a_2} f^{(1)}(x) \cos x \, dx + f(a_1) \cos a_1$$

$$- f^{(1)}(a_2) \sin a_2 - \int_{a_2}^{\infty} f^{(2)}(x) \sin x \, dx.$$ 

Repetition of this process finally gives

$$I(a) = \sum_{i=0}^{\infty} f^{(i)}(a_{i+1}) \cos \left[ a_{i+1} + i(\pi/2) \right]$$

$$+ \sum_{i=0}^{\infty} \int_{a_i}^{a_{i+1}} f^{(i)}(x) \sin \left[ x + i(\pi/2) \right] \, dx$$

where one may set

$$a_{i+1} \geq a_i; \quad a_0 = a.$$ 

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

$$S_i = \sum_{i=0}^{\infty} f^{(i)}(a_{i+1}) \cos \left[ a_{i+1} + i(\pi/2) \right]$$

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

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

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

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

as may always be done because of relation (2a). Now however the value of $f^{(2)}(a_2)$ 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 $S_i$ 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 $S_i$ provided only that

$$a_i'' \geq a_i'$$

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

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

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

\[
|f^{(i-1)}(x_i)| < |f^{(i-1)}(x)| \quad \text{for all } x_1 > x > A_i.
\]

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

\[
a_i > A_i.
\]

Because of equation (4a) then the relation

\[
|f^{(i-1)}(a_{i+1})/f^{(i-1)}(a_i)| < 1
\]

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

\[
|I_i| < \left| \int_{a_i}^{a_{i+1}} f^{(i)}(x) \, dx \right| = \left| f^{(i-1)}(a_{i+1}) - f^{(i-1)}(a_i) \right| =
\]

\[
|f^{(i-1)}(a_i) \left[ 1 - \frac{f^{(i-1)}(a_i+1)}{f^{(i-1)}(a_i)} \right] | < 2 |f^{(i-1)}(a_i)|; \quad i \neq 0
\]

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

\[
2 \sum_{i=1}^{\infty} |f^{(i-1)}(a_i)| = 2 \sum_{i=0}^{\infty} |f^{(i)}(a_{i+1})|
\]

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

\[
I(a) = \int_a^{\infty} x^{-k} \sin x \, dx; \quad k > 0.
\]

Here one may take (as will be shown)

\[
a_i = a + i\alpha
\]

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

\[
I(a) = S_1(a) + S_2(a)
\]

where

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

\[
S_2(a) = \sum_{i=1}^{\infty} \frac{(1)(k)(k+1) \cdots (k+i-2)}{(a+i\alpha)(k+i-1)} x^{-(k+i-1)} \cos [i(\pi/2 - x)] dx.
\]
Series $S_1$ converges if

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

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

or in other words if

$$\alpha > (1/e).$$

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 $\alpha$ 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 $\alpha$, 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 $\alpha$ 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

$$\int_0^\infty \frac{1}{(x^2 + 1)^{1/2}} dx = \pi.$$

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.

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