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

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

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

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

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

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

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

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

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

where one may set

\[
a_{i+1} > a_i; \quad a_0 = a.
\]

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

\[
S_1 = \sum_{i=0}^{\infty} f^{(i)}(a_{i+1})
\]

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

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

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

\[
|f^{(1)}(a_2)| < \rho \cdot |f^{(0)}(a_1)|
\]

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 \( S_1 \) 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 \( a_i = a_i', \text{ say} \) then the values \( a_i = a_i'' \) will also insure convergence of \( S_1 \) 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

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

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

\[
|I_i| < \int_{a_i}^{a_{i+1}} f^{(i)}(x)dx = |f^{(i-1)}(a_{i+1}) - f^{(i-1)}(a_i)| = |f^{(i-1)}(a_i)| 1 - \left[ f^{(i-1)}(a_i + 1)/f^{(i-1)}(a_i) \right] | < |f^{(i-1)}(a_i)|; \quad i \neq 0
\]

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

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

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

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

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

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

or in other words if

\[
\alpha > \frac{1}{e}.
\]

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

\[
\left(\frac{2}{\pi}\right) \sum_{i=1}^{\infty} \frac{(-1)^{i-1}}{(i-1)!} i^{\frac{i}{2}} x^{-i} \cos \left[i(\pi/2) - x\right] dx.
\]

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) \hspace{1cm} S_1 = .8727; \hspace{1cm} S_2 = .9762; \hspace{1cm} S_3 = .9951; \hspace{1cm} S_4 = .9988; \hspace{1cm} 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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