

Numerical Quadrature of Fourier Transform Integrals

I. Introduction. In applied mathematical problems the need frequently arises to evaluate numerically integrals of the form

$$(1a) \quad S(x) = \int_0^{\infty} \phi(k) \sin kx dk$$

or

$$(1b) \quad C(x) = \int_0^{\infty} \psi(k) \cos kx dk.$$

In some cases the function $\phi(k)$ or $\psi(k)$ is given by a closed expression which is too complicated to permit a sufficiently accurate analytic evaluation of the integral for the entire range of the parameter x . In other cases $\phi(k)$ or $\psi(k)$ may be available only in numerical form.

The conventional methods of numerical quadrature (e.g., Simpson's rule) are not suitable for evaluation of the above integrals when x is large. There are two reasons for the failure of the standard methods in this case. First, because of the rapid oscillation of the trigonometric function when x is large the integrand cannot be accurately approximated by simple polynomials unless undesirably small intervals of integration are chosen. Secondly, the extremely strong cancellation between the contributions to the integral from regions where the trigonometric function is positive and regions where it is negative tends to accentuate the errors in the conventional integration procedures.

Filon [1] and Luke [2] have suggested methods of integration which avoid the first difficulty by using polynomial approximations for $\phi(k)$ or $\psi(k)$ rather than for the entire integrand. In this note we shall discuss a new scheme which attempts to alleviate the second difficulty as well. In this scheme all half cycles of the trigonometric functions are treated in an identical manner so that no cancellation errors arise. The integration scheme for the individual half cycles is based on a Gaussian type integration procedure [3] which minimizes the error in the final result for a given number of integration points per half cycle. In developing the integration formulas for the individual half cycles, it is imagined that the integrals in (1a) and (1b) are evaluated by first performing the sum of the integrand at corresponding points in all half cycles and then integrating the result over a single half cycle. The sum over corresponding points in all the half cycles possesses certain properties which, particularly for large x , enable the final integral to be accurately evaluated with a small number of points per half cycle.

In the actual numerical evaluation of the integral, the integrations are first performed over the individual half cycles, and then the total contributions of the various half cycles are summed. Although the integration formulas are not accurate for the individual half cycles, most of the error cancels when the sum over half cycles is performed (see section V).

In performing the sum over half cycles, the standard techniques for accelerating the convergence of the sums of an oscillating series can be employed. This

greatly reduces the number of half cycles which must be considered to obtain a final result of specified accuracy.

A disadvantage of the method is that the values of k at which $\phi(k)$ or $\psi(k)$ must be evaluated depends on the value of the parameter x . Hence the method is most useful when results are needed for only a few values of x . If results are needed for a large number of values of x , the Gaussian integration feature could be sacrificed without serious loss in accuracy. This would enable the points at which the integrand is to be evaluated to be spaced uniformly instead of at irregular intervals as in the Gaussian procedure. It is, of course, still necessary for the interval in k to be an integral fraction of π/x , but the integral can be evaluated for several values of x with the same spacing in k . Only the simplest example of the uniform spacing method, i.e., one point per half cycle, will be specifically treated in this note. The generalization of the uniform spacing method to a greater number of points is, however, straightforward. The discussion in the following sections indicates that, although the uniform spacing method is by no means as accurate as the Gaussian procedure, the loss in accuracy with a corresponding number of integration points may not be serious for practical applications.

It must be recognized that although the method described here is designed to reduce cancellation errors associated with the integration formulas themselves, the method does not eliminate the possibility of cancellation errors in the numerical application of the formulas. Therefore, the numerical values of $\phi(k)$ or $\psi(k)$ which are used in the evaluation must ordinarily be accurate to a number of significant figures equal to the number required in the final answer plus the number lost due to cancellation. There are, however, circumstances in which consistent approximations may be made in the calculation of $\phi(k)$ or $\psi(k)$ which do not introduce as large an error in the final result as would be expected on the basis of a consideration of significant figures. These approximations may usually be regarded as corresponding to the replacement of the actual physical problem by a slightly modified problem which, on physical grounds, must lead to almost the same final result. It is, of course, necessary to retain as many significant figures in the calculation of $\phi(k)$ or $\psi(k)$ in the modified problem as would be necessary on the basis of elementary considerations. This is true despite the fact that the integrand as calculated in the modified problem may agree with the correct integrand to far fewer significant figures than must be retained in the evaluation of the integral.

In many cases the strong cancellation occurring in integrals of the type appearing in (1a) and (1b) may be interpreted as resulting from the fact that there is a saddle point of the integrand in the complex k -plane which, for large x , is far removed from the real axis. Hence the ideal method of numerically evaluating the integral would be to integrate along a path in the complex k -plane passing through the saddle point. It is interesting to note that one is led to a consideration of complex values of k by the following independent argument. One expands the function $\phi(k)$ or $\psi(k)$ in a power series in the variable

$$(2) \quad u = (1 + k^2 L^2)^{-1},$$

where L^2 is a suitably chosen parameter. If one then applies the Gaussian integration procedure to the infinite integrals in (1a) or (1b) by using polynomials in the variable u , one finds that when x is large the optimum points for evaluation of the integrand cluster around the point i/L in the k -plane. If L has been chosen correctly, this point is, in turn, close to the saddle point of the complex integral. Although this method of numerically inverting Fourier transforms is in principle more powerful than the one considered above, it is probably less practical, mainly because of the need to evaluate the integrand for complex values of k .

II. Preliminary algebraic manipulation. It is necessary to express the integrals (1a) and (1b) as integrations over a single half cycle of the integrand, summed then over all half cycles, in order to apply the methods outlined in section I. However, in order to simplify the derivation of the method the order of summation and integration are interchanged, i.e., the summation is performed first. The justification of the interchanging of order of summation and integration is given in section V.

We begin by making the transformation

$$(3a) \quad y = kx/\pi - \frac{1}{2}$$

in (1a), and

$$(3b) \quad u = kx/\pi$$

in (1b). For purposes of the derivation, it is convenient to extend the integrals to the range $-\infty \leq k \leq +\infty$, which may be done if the definitions of the functions ϕ and ψ are extended to negative values of k by the definitions

$$(4a) \quad \phi(-k) = -\phi(k),$$

and

$$(4b) \quad \psi(-k) = \psi(k).$$

In most applications of interest, the functions thus defined are regular in the range $k = -\infty$ to $+\infty$. (Note that the restrictions implied on $\psi(k)$ and $\phi(k)$, namely $\phi(0) = 0$ and $\psi'(0) = 0$ are physically reasonable. For example, if (1a) arose from the inversion of a three-dimensional Fourier transform $f(k)$, then $\phi(k) \sim kf(k)$.)

Applying (3) and (4) to (1) leads to

$$(5a) \quad S(x) = \frac{\pi}{2x} \int_{-\frac{1}{2}}^{\frac{1}{2}} \cos \pi y \sigma(y, x) dy,$$

and

$$(5b) \quad C(x) = \frac{\pi}{2x} \int_{-\frac{1}{2}}^{\frac{1}{2}} \cos \pi u \gamma(u, x) du,$$

where

$$(6a) \quad \sigma(y, x) = \sum_{n=-\infty}^{+\infty} (-)^n \phi\left(\frac{\pi}{x} \left[y + n + \frac{1}{2}\right]\right),$$

and

$$(6b) \quad \gamma(u, x) = \sum_{n=-\infty}^{+\infty} (-)^n \psi\left(\frac{\pi}{x} [u + n]\right).$$

The function $\sigma(y, x)$ has the following properties [all the subsequent remarks apply equally well to $\gamma(y, x)$] as may be seen from (4) (6):

- (a) $\sigma(y, x) = \sigma(-y, x)$,
- (b) $\sigma(\frac{1}{2}, x) = \sigma(-\frac{1}{2}, x) = 0$
- (c) $\sigma(y + n, x) = (-)^n \sigma(y, x)$,
- (d) σ is regular, $-\frac{1}{2} \leq y \leq \frac{1}{2}$ if $\phi(k)$ is regular for $-\infty \leq k \leq +\infty$.

Because of these properties, σ (and γ) can be expanded in Fourier series of the form

$$(7a) \quad \sigma(y, x) = \sum_{n=0}^{\infty} a_n(x) \cos(2n+1)\pi y,$$

or, since $\cos n\theta$ is a polynomial of exact degree in $\cos \theta$,

$$(7b) \quad \sigma(y, x) = \cos \pi y \sum_{n=0}^{\infty} \alpha_n(x) \cos^{2n} \pi y,$$

with a similar expression for γ .

III. Gaussian integration procedure. Substitution of (7b) in (5a) gives

$$(8) \quad S(x) = \frac{\pi}{2x} \int_{-\frac{1}{2}}^{\frac{1}{2}} \cos^2 \pi y \sum_{n=0}^{\infty} \alpha_n(x) \cos^{2n} \pi y dy.$$

In order to integrate such an integral as accurately as possible, the Gaussian integration procedure is employed [3]. A set of polynomials in $\cos^2 \pi y$ orthogonal on the interval $(-\frac{1}{2}, \frac{1}{2})$ with weighting function $\cos^2 \pi y$ is found. Representing these polynomials by $\Gamma_n(\cos \pi y)$, one has

$$(9) \quad \int_{-\frac{1}{2}}^{\frac{1}{2}} \cos^2 \pi y \Gamma_n(\cos \pi y) \Gamma_m(\cos \pi y) dy = 0 \quad \text{for } n \neq m.$$

The polynomials in $\cos^2 \pi y$ which obey (9) may easily be shown to be related to the Chebyshev polynomials of the first kind [4], $T_n(x)$:

$$(10) \quad \begin{aligned} \Gamma_n(\cos \pi y) &= (\cos \pi y)^{-1} T_{2n+1}(\cos \pi y) \\ &= (\cos \pi y)^{-1} \cos(2n+1)\pi y. \end{aligned}$$

See, for example, [4]. (The authors are indebted to the referee for pointing out this relationship.) The $2N$ -point Gaussian quadrature formula is simply

$$(11) \quad \int_{-\frac{1}{2}}^{\frac{1}{2}} \cos \pi y \sigma(y, x) dy = \sum_{j=1}^N \frac{2W_j^{(N)}}{\cos \pi y_j^{(N)}} \sigma(y_j^{(N)}, x),$$

where the $y_j^{(N)}$ are the zeros of $\Gamma_N(\cos \pi y)$:

$$(12) \quad y_j^{(N)} = \frac{2j-1}{2(2N+1)}, \quad j = 1, 2, \dots, N,$$

and the W_j are the so-called Christoffel numbers. (Since $\sigma(y, x)$ is an even function in y , the contribution to the numerical integration from $-y_j$ is equal to the contribution from $+y_j$; furthermore, it is easy to show that the Christoffel number associated with $+y_j$ is equal to the one associated with $-y_j$. For this reason, we consider only the positive zeros of $\Gamma_N(\cos \pi y)$, and introduce the factor of two on the right side of (11). Thus, although the integrand is evaluated at only N points, the formula is called a $2N$ -point formula. In section V, however, where the order of integration and summation is reversed for numerical convenience, it is necessary to evaluate the integrand at both $\pm y_j$, which gives the numerical integration formula as stated there a slightly different appearance.)

Note the factor of $(\cos \pi y_j^{(N)})^{-1}$ in (11), which arises from the fact that a $\cos \pi y$ was factored out of $\sigma(y, x)$ in (8), and the weighting factor $\cos^2 \pi y$ was used, although the original integrand involved only the first power of $\cos \pi y$.

The $W_j^{(N)}$ may be found by requiring that (11) give an exact answer if $\frac{\sigma(y, x)}{\cos \pi y}$ is a polynomial of degree up to and including $N-1$ in $\cos^2 \pi y$. It then follows automatically that (11) will also give an exact result for polynomials from degree N to $2N-1$ inclusive in $\cos^2 \pi y$. Since

$$(13) \quad \int_{-\pi/2}^{\pi/2} \cos^{2\lambda} y dy = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\lambda + \frac{1}{2})}{\Gamma(\lambda + 1)},$$

then the $W_j^{(N)}$ are the solutions of the N simultaneous equations:

$$(14) \quad \frac{1}{\sqrt{\pi}} \frac{\Gamma(\lambda + \frac{1}{2})}{\Gamma(\lambda + 1)} = 2 \sum_{j=1}^N \cos^{2\lambda-2} \left(\frac{[2j-1]\pi}{2[2N+1]} \right) W_j^{(N)},$$

$$\lambda = 1, 2, \dots, N.$$

(It is also possible to obtain a general closed expression for the Christoffel numbers [3], although the actual evaluations of the Christoffel numbers are just as simple if (14) is used directly.)

The y_j and W_j are given below for the two- and four-point formulas:

(a) Two-point Formula ($N = 1$):

$$y_1 = \frac{1}{6}$$

$$\cos \pi y_1 = \frac{1}{2}\sqrt{3}$$

$$W_1 = \frac{1}{4}$$

(b) Four-point Formula ($N = 2$):

$$y_1 = \frac{3}{10} \quad y_2 = \frac{1}{10}$$

$$\cos \pi y_1 = 0.58778 \, 52 \quad \cos \pi y_2 = 0.95105 \, 65$$

$$W_1 = 0.06909 \, 832, \quad W_2 = 0.18090 \, 169.$$

It will sometimes be found that a one-point formula gives sufficient accuracy (see section IV). This formula gives an exact answer only if $\frac{\sigma(y, x)}{\cos \pi y}$ is independent of y . In this special case, (11) becomes

$$(15) \quad \int_{-\frac{1}{2}}^{\frac{1}{2}} \cos \pi y \sigma(y, x) dy = \frac{1}{2} \sigma(0, x).$$

IV. Choice of N . The number of points which must be used in the Gaussian procedure in order to obtain a numerical answer within a required degree of accuracy may be shown to depend upon the magnitude of x . From the arguments given here, a qualitative dependence of the error introduced by the N -point formula may be obtained as a function of x . Consider the example

$$(16) \quad \psi(k) = (1 + L^2 k^2)^{-1}.$$

The integral (1b) may be evaluated analytically, yielding

$$(17) \quad C(x) = \frac{\pi}{2L} e^{-x^*}, \quad x^* = x/L.$$

The $2N$ -point quadrature formula gives for $C(x)$,

$$(18) \quad C(x) = \frac{\pi}{2x} \sum_{j=1}^N \frac{2W_j^{(N)}}{\cos \pi y_j^{(N)}} \gamma(y_j^{(N)}, x),$$

where

$$(19a) \quad \gamma(y_j^{(N)}, x) = \sum_{n=-\infty}^{+\infty} (-)^n \frac{x^2}{x^2 + L^2 \pi^2 (y_j^{(N)} + n)^2} \\ = \frac{x^* \sinh x^* \cos \pi y_j^{(N)}}{\sin^2 \pi y_j^{(N)} \cosh^2 x^* + \cos^2 \pi y_j^{(N)} \sinh^2 x^*},$$

$$(19b) \quad \frac{\gamma(y_j^{(N)}, x)}{\cos \pi y_j^{(N)}} = 2x^* [e^{-x^*} - e^{-3x^*}] [1 + (4 \cos^2 \pi y_j^{(N)} - 2)e^{-2x^*} + \dots].$$

Thus, it is seen from (19b) that for large x , (7) is rapidly convergent. From (18) and (19b), one sees that in the limit of x large

$$(20) \quad C(x) = \frac{\pi}{2L} e^{-x^*} + O[e^{-3x^*}],$$

independent of N , so that even the one-point formula may be used. As x decreases, however, it is necessary to go to larger values of N .

In Figure 1, the error introduced into the evaluation of $C(x)$ by the one-, two-, and three-point formulas with $\psi(k)$ given by (16) is plotted as a function of x^* , where the numerical evaluation of $C(x)$ is obtained from (18) in conjunction with

(17a). Note that the error depends on the ratio x/L (i.e., x^*) since this quantity determines how much the integrand decreases in one cycle of the trigonometric factor. When the rate of decrease is small (i.e., x^* is large) the required number of integration points per half cycle is small.

V. Outline of numerical procedure and discussion. In order to evaluate the sum appearing in (11), it is convenient to change the order of summation and (numerical) integration. That is, the order of the two sums on the right side of

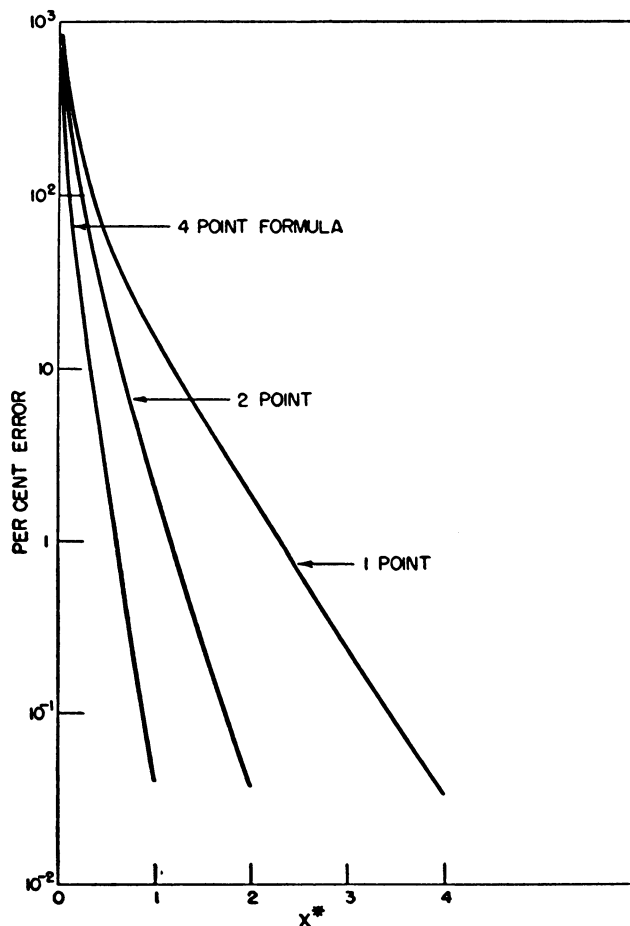


FIG. 1. Per Cent Error in Integration Schemes as a Function of x^* .

(11) are reversed. This procedure corresponds to a separate integration of every half cycle, with a subsequent summation over the cycles, as is described in section I. It may easily be shown that this reversal may be made since if the integrals (1) exist, then the series (6) for $\sigma(y)$ and $\gamma(y)$ converge uniformly on the range $-\frac{1}{2} \leq y \leq \frac{1}{2}$. (The only restriction on $\phi(k)$ (and $\psi(k)$) is that there exist a k_0 such that $\phi(k_1) > \phi(k_2)$ if $k_0 \leq k_1 \leq k_2$.) It is also convenient to change the formulation slightly so that the half-cycle sums are carried out from zero to infinity.

We define

$$(21a) \quad S(x) = \frac{\pi}{x} \sum_{n=0}^{\infty} S_n(x),$$

and

$$(21b) \quad C(x) = \frac{\pi}{x} \left[\frac{1}{2} C_0(x) + \sum_{n=1}^{\infty} C_n(x) \right],$$

with

$$\begin{aligned} (22a) \quad S_n(x) &= (-)^n \int_{-\frac{1}{2}}^{\frac{1}{2}} \phi \left[\frac{\pi}{x} (y + n + \tfrac{1}{2}) \right] \cos \pi y dy \\ &= (-)^n \sum_{j=1}^N \frac{W_j^{(N)}}{\cos \pi y_j^{(N)}} \\ &\quad \times \left\{ \phi \left(\frac{\pi}{x} [y_j^{(N)} + n + \tfrac{1}{2}] \right) + \phi \left(\frac{\pi}{x} [-y_j^{(N)} + n + \tfrac{1}{2}] \right) \right\}, \end{aligned}$$

and

$$\begin{aligned} (22b) \quad C_n(x) &= (-)^n \int_{-\frac{1}{2}}^{\frac{1}{2}} \psi \left(\frac{\pi}{x} [u + n] \right) \cos \pi u du \\ &= (-)^n \sum_{j=1}^N \frac{W_j^{(N)}}{\cos \pi u_j^{(N)}} \\ &\quad \times \left\{ \psi \left(\frac{\pi}{x} [u_j^{(N)} + n] \right) + \psi \left(\frac{\pi}{x} [-u_j^{(N)} + n] \right) \right\}. \end{aligned}$$

In order to sum the series in (21) any standard method [5] [6] for the summation of oscillating series may be employed. A method suggested to the authors by Mrs. M. Ray has been found to be quite convenient; it appears to be sufficiently accurate for most purposes, and is quite simple. The method is to form the sequence of partial sums,

$$(23) \quad \beta_n = \sum_{\alpha=0}^n S_{\alpha}(x),$$

so that

$$(24) \quad S(x) = \frac{\pi}{x} \lim_{n \rightarrow \infty} \beta_n.$$

The limit of the sequence $\beta_0, \beta_1, \dots, \beta_n, \dots$ is then found by the "averaging" technique. That is, we define

$$\begin{aligned} (25) \quad a_1^{(n)} &= \tfrac{1}{2} (\beta_n + \beta_{n+1}), \\ a_2^{(n)} &= \tfrac{1}{2} (a_1^{(n)} + a_1^{(n+1)}), \end{aligned}$$

etc.,

$$(26) \quad \lim_{n \rightarrow \infty} \beta_n = \lim_{j \rightarrow \infty} a_j.$$

The sequence of a_j 's in general converges much more rapidly than does the sequence of β_n 's. (Note that a_j , as defined by (25), is given in [7] (Exercise 120, p. 271), as the j -th partial sum of a series equivalent to the original oscillating series. Thus, our procedure corresponds to summing the equivalent series which is defined in [7] (paragraph 144, p. 244). The summation procedure described here is useful because the equivalent series converges more rapidly than the original series. Still faster convergence could presumably be obtained in typical cases by the application of the more refined procedures discussed in the references given in [6] and [7].)

TABLE I. *Replica of Portion of Work Sheet, Demonstrating a Convenient Method of Setting Up Calculations*

n	$\phi\left(\frac{\pi}{x}[y_1 + n + \frac{1}{2}]\right)$	$S_n = (-)^n W_1 \phi\left(\frac{\pi}{x}[y_1 + n + \frac{1}{2}]\right)$	$\beta_n = \sum_{j=0}^n S_j$	$a_1^{(n)} = \frac{1}{2}(\beta_n + \beta_{n+1})$
\vdots	\vdots	\vdots	\vdots	\vdots
10	0.27763 71	+0.13881 86	+0.06689 27	$+2.6191 \times 10^{-3}$
11	0.25709 43	-0.12854 72	-0.06165 45	-1.8693×10^{-3}
12	0.23914 07	+0.11957 04	+0.05791 59	$+2.0741 \times 10^{-3}$
13	0.22336 71	-0.11168 36	-0.05376 77	-1.4098×10^{-3}
14	0.20943 14	+0.10471 57	+0.05094 80	$+1.6853 \times 10^{-3}$
15	0.19705 09	-0.09852 545	-0.04757 74	-1.0791×10^{-3}
16	0.18599 31	+0.09299 66	+0.04541 92	

Table I is the replica of a portion of a work sheet in which the integral

$$(27) \quad S(x) = \int_0^\infty \frac{k}{1+k^2} \sin kx dk = \frac{1}{2}\pi e^{-x},$$

was evaluated by the single-point formula, with $x = 10$, demonstrating a convenient method of setting up the calculation. In Table II, the summation process is illustrated for this case. The criterion for ending the calculation is the near constancy of the last two or more terms in the upper diagonal of Table II ($a_j^{(n)} \cong a_{j+1}^{(n)}$)

TABLE II. *Illustration of Summation Procedure*

n	$a_1^{(n)} \times 10^3$	$a_2^{(n)} \times 10^4$	$a_3^{(n)} \times 10^4$	$a_4^{(n)} \times 10^4$	$a_5^{(n)} \times 10^4$
10	+2.6191				
11	-1.8693	3.749			
12	+2.0741	1.024	2.386	2.271	
13	-1.4098	3.322	2.173	2.270	2.270
14	+1.6853	1.378	2.350		
15	-1.0791	3.031	2.204		
16					

which indicates the sequence has closely approached its limit. We then take

$$S(x) \cong \frac{\pi}{x} a_5^{(n)}.$$

The numerical result for $S(x)$ is 7.131×10^{-5} , compared to the rigorous value of 7.1314×10^{-5} . Since the error introduced by the quadrature rule is only of the order $e^{-2x} = e^{-20}$, the main error in this procedure is introduced in the summation process, during which significant figures are lost. Thus, the numerical result obtained here agrees with the analytical result to as many significant figures as were retained during the numerical procedure. However, three of the seven figures to which $\phi(k)$ was originally evaluated were lost during integration.

The same integral has been treated numerically by Simpson's and Filon's methods, and it has been found that in order to obtain accuracy comparable to that obtainable by the method described here the integrand must be evaluated at least 10 times as many points.

The tables and graph in this paper were prepared by Miss D. M. Keaveney.

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Formulas for the Partial Summation of Series

1. **Introduction.** The paper gives a table of the coefficients $A_m(n)$ in the "partial" summation formula $S_n \doteq \sum_{m=4}^{10} A_m(n)S_m$. The coefficients $A_m(n)$, $m = 4(1)10$, are tabulated exactly in the fractional form $C_m(n)/D(n)$ for $n = 11(1)50(5)100(10)200(50)500(100)1000$. For every n , except 47, $D(n)$ is the least integer containing no more than ten digits exclusive of final zeros, to permit ready division on a ten-bank calculating machine using $S_n \doteq \left[\sum_{m=4}^{10} C_m(n)S_m \right] / D(n)$.

The purpose of $A_m(n)$ is the calculation of the sum of n terms of a slowly convergent series, or, more generally, the evaluation of the n -th term of a sequence S_m which is either slowly convergent or asymptotically characterized by $S_m \sim f(m)$ (convergent or divergent), in such a manner that the auxiliary sequence $S_m/f(m)$ is slowly convergent. The formula for S_n was obtained by Lagrangian extrapolation upon S_m considered as a polynomial in $1/m$, based upon the last 7 values of