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Note

The Evaluation of Integrals with Oscillatory Integrands*

We present here an extension to Filon's method for the evaluation of oscillatory integrals with infinite limits. The method amounts to producing an asymptotic expansion for the original integral. The qualitative relevance of our results is indicated.

There are a few methods available for the evaluation of integrals of the form

$$I(r) = \int_0^\infty f(k) \sin^2 k r \, dk, \qquad (1)$$

which frequently occur in investigations in mathematical physics.

The methods adopted by Hurwitz and Zweifel [1], Hurwitz, Pfeifer, and Zweifel [2], Saenger [3], and Balbine and Franklin [4], converting the infinite integral into a summation by subdividing the range and performing the integration between successive zeros of $\frac{\sin kr}{\cos kr}$ prove to be not completely satisfactory in all cases.

This is particularly true for cases where the approximating series does not converge rapidly.

The same applies to Longmann's [5] approach in which he used a variation of Euler's transformation to accelerate convergence.

A further development of this approach was proposed by Alaylioglou, Evans, and Heyslop [6] who investigated the use of the more general nonlinear transformation of Shank [7] and reported quite satisfactory results. Perhaps, a disadvantage of this approach (and indeed of all subdivision/acceleration algorithms) is that the integration limits (a_n, a_{n+1}) depend on the parameter r, thus the Gaussian-Legendre Integration points have to be retransformed for each of its values. This is not apparent when one seeks to evaluate the integral (1) for a few values of r, but it might become a laborious task when r assumes a sufficiently large number of values.

The original method, proposed by Filon [8], of approximating f(k) with a polymonial of a low degree does not provide for the evaluation of integrals of infinite range and cannot be applied directly.

* This paper is based on part of a MS. thesis by G. Pantis, University of South Africa, unpublished.

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In this paper we shall show that Filon's approach gives reasonably accurate results if an asymptotic expansion of the original integral is performed. The basic idea is to write the integral (1).

$$I(r) = \int_0^\infty f(k) \sin kr \, dk = I_1(r) + I_2(r), \tag{2}$$

where

$$I_1(r) = \int_0^\alpha f(k) \sin kr \, dk, \tag{3}$$

$$I_2(r) = \int_{\alpha}^{\infty} f(k) \sin kr \, dk, \qquad (4)$$

and use the Filon's method for the evaluation of the term $I_1(r)$. Then, provided that the function f(k) is suitably behaved, (i.e., f(k) decreases as $(1/k^p)$ $(p \ge 1)$ with increasing k) the term $I_2(r)$ can be accurately approximated by integrating by parts. Thus Eq. (4) simply reads:

....

$$I_{2}(r) = \left(\sum_{\lambda=0}^{\mu} \frac{(\lambda)}{f(k)} \frac{(\lambda)}{r^{2\lambda+1}}\right)_{k=\alpha} + \int_{\alpha}^{\infty} \frac{(\mu+1)}{f(k)} \frac{(\mu)}{\cos kr} dk,$$
(5)

where the notation (λ) indicates the order of the derivative with respect to k. Clearly $f^{(0)} = f$.

In most cases in practice the $\mu = 1$ or $\mu = 2$ approximations will be sufficiently accurate whereby the integral term of Eq. (5) can be completely omitted. For example consider the function

$$f(k) = k/(1+k^2).$$
 (6)

$$A_1(r) = (2/\pi) \int_0^\infty \frac{k}{(1+k^2)} \sin kr \, dk = e^{-r} = 0.3678794..., \quad \text{at} \quad r = 1.$$
 (7)

The $\mu = 2$ approximation gives

$$A_1(1) = 0.3678793...,$$
 for $\alpha = 100$, and $T_N = 700$

 T_N is the number of evaluation points in the Filon routine. It is significantly smaller for functions f(k) converging faster than Eq. (6). This can be seen by considering the integral

$$A_2(r) = \int_{\pi}^{\infty} x^{-2} \sin xr \, dx = , -ci(\pi) = -0.0736681, \quad \text{at} \quad r = 1.$$
 (8)

In the $\mu = 1$ approximation we get

$$A_2(1) = -0.0736681$$
 for $\alpha = 30 + \pi$, $T_N = 200$.

As a final example consider the integral

$$A_{3}(r) = \int_{0}^{\infty} x^{-1} e^{-x/2} \sin xr \, dx = \tan^{-1}(2r) = 1.107148718..., \quad \text{at} \quad r = 1.$$
 (9)

In the $\mu = 1$ approximation we get

$$A_3(1) = 1.107149...,$$
 for $\alpha = 20$ and $T_N = 100,$

or

$$A_3(1) = 1.107148718$$
, for $\alpha = 30$ and $T_N = 500$,

which is accurate to ten digits.

The implication of these results is that the accuracy of this approach can be further improved by increasing T_N or by increasing α and T_N simultaneously.

Equation (5) was derived here for easy presentation. In many nuclear physics problems, however, integrals of the form (1) frequently occur, where the functions f(k) are not known analytically but are only given at a number of points k_i . For example we encountered recently the problem of the evaluation of Nonlocal Potentials and their Equivalent Local ones, from the scattering phase shift. In such cases, it is preferable to divide beforehand the range of the integration $(0, \alpha)$, in Eq. (3), into a number of t unequal parts α_i , such that

$$\alpha = \sum_{i=0}^{t} \alpha_i = \sum_{i=0}^{t} (p_i, p_{i+1}),$$
(10)

and then apply the Filon routine separately, viz,

$$I_{1}(r) = \sum_{i=0}^{t} \int_{p_{i}}^{p_{i+1}} f(k) \sin kr \, dk.$$
 (11)

This has the advantage that should the function f(k) not decrease uniformly (monotonically), but exhibit one or more maxima in a particular interval $\alpha_i = (p_i, p_{i+1})$, a large number of evaluation points N_i can be used in that interval, whilst this same number of points need not be retained throughout the interval $(0, \alpha)$. We should note here that this approach was found useful in computing the *D*-wave function of the deuteron [9]

$$W_{D}(r) = \int_{0}^{\infty} j_{l}(k, r) \, kf(k) \, dk, \qquad l = 2, \tag{12}$$

where $j_l(k, r)$ are the usual Bessel's functions. As a practical example, we consider again the function f(k) Eq. (6). The results are shown in Table I, where $\alpha = 400$ and 600 for the same total number of evaluation points $T_N = 144$.

We noticed that this approach is very useful for functions f(k) which do not decrease rapidly and thus the interval $(0, \alpha)$ assumes large values. Furthermore only one or two terms ($\mu = 0$ or 1) are needed to provide a sufficiently high accuracy, though with a much smaller number of evaluation points T_N .

t	p_i	r	μ	$I(r)_{\rm Ex} - I(r)_{\rm Num}$	N_i
			0	0.2 × 10 ⁻⁵	
		1.0 1 2 100, 400	1	$0.9 imes 10^{-6}$	
	0 4 16 20 100 400		$0.9 imes 10^{-6}$	50 40 14 20 20	
4	0, 4, 16, 30, 100, 400		0	0.1 × 10 ⁶	50, 40, 14, 20, 20
			1	$0.9 imes10^{-7}$	
			2	0.9×10^{-7}	
		$5, 30, 100, 600 \qquad \begin{array}{cccc} 1.0 & 1 & 0.4 \times 10^{-1} \\ 2 & 0.4 \times 10^{-1} \\ \hline & 0 & 0.9 \times 10^{-1} \\ 10.0 & 1 & 0.8 \times 10^{-1} \end{array}$	0	0.5 × 10 ⁻⁶	
			1	$0.4 imes10^{-6}$	
	0 4 16 20 100 600		$0.4 imes 10^{-6}$	50, 40, 14, 20, 20	
4	0, 4, 10, 30, 100, 600		0.9 × 10 ⁻⁷		
			$0.8 imes10^{-7}$		
			2	0.8×10^{-7}	

TABLE I	TABLI			
Numerical Error in the Evaluation of $A_1(r)$	Numerical			

It should be mentioned that the accuracy of our method increases as the parameter r increases. This is readily explained: The terms of the series that are omitted, are divided by $r^{2\lambda+1}$ so that they become zero as r becomes large.

As far as time of computation is concerned, the evaluation of the function f(k) at the integration points is the most time consuming part. This means that for calculation at a single value of r the subroutines described here take longer than those of other conventional methods. If, however, several values of r are needed, these subroutines become very fast, since the evaluation of the function f(k) need only be done once. For example we note, that for the function (6) these subroutines take 30 seconds, for 40 values of r, on a Burroughs 5700 computer.

In conclusion it is noted that the method outlined here is a useful tool for

evaluating integrals of the form (12) and especially for such functions f(k) which are not known analytically. Our method can thus be regarded as a useful supplement to the normal Filon routine, for an infinite integration range.

Appendix

All formulae associated with the Filon's method are given in Filon's original paper [8]. Here we shall briefly discuss the case of an integral of the form

$$I(r) = \int_0^\infty \frac{\sin kr}{k} f(k) \, dk, \quad f(k) \neq 0 \text{ at } k = 0.$$
 (A.1)

A formula for the evaluation of singular integrals such as (A.1) was also devised by Filon. We noticed, however, that our approach provides for the evaluation of (A.1) without the use of this formula: For, if the interval (p_0, p_1) is chosen small (say 1.0) and a large number of evaluation points is taken, the coefficient α in Filon's Eq. (16) is almost equal to zero, so that the singular term (in Filon's Eq. (15)) can be set equal to zero without significant loss of accuracy.

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References

- 1. H. HURWITZ AND P. F. ZWEIFEL, M.T.A.C. 10 (1956), 140.
- 2. H. HURWITZ, R. A. PFEIFER, AND P. F. ZWEIFEL, M.T.A.C. 13 (1959), 87.
- 3. A. SAENGER, J. Math. Anal. Appl. 8 (1964), 1.
- 4. G. BALBINE AND J. N. FRANKLIN, Math. Comp. 20 (1966), 570.
- 5. I. M. LONGMAN, Math. Comp. 14 (1960), 53.
- 6. A. ALAYLIOGLOU, G. EVANS, AND J. HYSLOP, J. Computational Phys. 13 (1973), 433.
- 7. D. SHANKS, J. Math. and Phys. 34 (1955), 1.
- 8. L. N. FILON, Proc. Roy. Soc. Ser. A (London) 49 (1928), 38.
- 9. N. J. MCGURK, H. DE GROOT, H. FIEDELDEY, AND H. J. BOERSMA, Phys. Lett. B 49 (1974), 13.

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