Fourier or Bessel transformations of highly oscillatory functions

1992 J. Phys. A: Math. Gen. 25 6755

(http://iopscience.iop.org/0305-4470/25/24/026)

J. Phys. A: Math. Gen. 25 (1992) 6755–6760. Printed in the UK

Fourier or Bessel transformations of highly oscillatory functions

Q Haider† and L C Liu‡

† Physics Department, Fordham University, Bronx, New York 10458, USA
‡ Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

Received 22 May 1992, in final form 25 August 1992

Abstract. An algorithm for integral transformation of highly oscillatory functions is presented. It is a generalization of the 'standard' Gaussian quadrature method but has the virtue that the usual tedious tests of convergence of the numerical results is not necessary. The effectiveness and accuracy of the algorithm is tested for both large arguments and higher orders of the Bessel function.

1. Introduction

In many physics and chemistry problems, one frequently encounters integral transforms (e.g. Fourier or Bessel transforms) of the form $f(q) = \int j_n(qx)g(x)x^2\,dx$, where $j_n(x)$ is the spherical Bessel function of order n and g is a function depending on the specificity of the problem. In the case of excitations of a molecule, atom or nucleus, $g(x)$ will be a transition density distribution. The function $|f(q)|^2$ then represents the response of the matter to external stimulation, or the momentum transfer q. In most of the cases, these transformations cannot be done analytically and one has to rely entirely on numerical methods. However, for large q or higher order Bessel functions (i.e. large n), the integrand becomes highly oscillatory and thereby presents serious difficulties in obtaining numerical convergence of the integration.

Out of a variety of applicable numerical integration methods, the one most commonly used for doing integral transformation is the 'standard' Gaussian quadrature method [1]. In using the Gaussian method, one has to be extremely careful in choosing the number of Gaussian points and the corresponding weights. *A priori* it is very difficult to determine how many points and weights should be used in order to achieve convergence to the exact result. This problem becomes more acute if the integrand cannot be cast in an analytical form and, as mentioned earlier, oscillates a lot.

This paper describes and demonstrates an algorithm, termed the 'partitioned' Gaussian method (PGM), that is free from the tedious tests of convergence. The method may be viewed as a special case of adaptive quadrature [2] and is particularly useful if the function that is to be integrated has a large number of zeros. The algorithm can be easily implemented on personal computers and used for solving various kinds of physics or chemistry problems [3]. The method is described briefly in section 2. Numerical examples are given in section 3 and in section 4, the results are summarized.

0305-4470/92/246755+06$07.50

2. 'Partitioned' Gaussian method

We are interested in numerical evaluation of integrals of the type

$$f(y) = \int_{x_0}^{x_m} K(x,y)g(x)\,\mathrm{d}x \tag{1}$$

where K is the kernel and $g(x)$ is the function that is to be integral transformed. The upper limit (x_m) of the integration could be either finite or infinite. In most physics and chemistry problems, $x_0 = 0$ and $x_m = \infty$, or $x_0 = 0$ and $x_m = a$, where a is a constant. In the first case, the function $g(x)$ usually goes to zero exponentially at large x. Very often, K is a Bessel function or functions related to Bessel function [4]. Since Bessel functions are oscillatory, the integrand $I(x,y) = K(x,y)g(x)$ will also be oscillatory even when $g(x)$ is smooth.

The essence of the PGM that is being proposed in this paper is to carry out the integration in equation (1) separately for each oscillation segment of $I(x,y)$. We form, therefore, the following sum:

$$f(y) = \sum_{i=1}^{N+1} \sum_{j=1}^{N_g} I(x_j, y)w_j \tag{2}$$

where N_g is the number of Gaussian points in each segment of integration $[X_{i-1}, X_i]$. The X_i $(i = 1,2,\ldots,N)$ are the location of the zeros of the integrand, N being the number of zeros. Furthermore, $X_0 \equiv x_0$ and $X_{N+1} \equiv x_m$. The x_j and w_j are, respectively, the corresponding abscissae and weights to be used in each segment. The number of zeros and X_i can be determined easily by searching with a very fine mesh size (ϵ) where the product $I(x,y)I(x+\epsilon,y)$ is less than zero. In the case $x_m = \infty$, we choose a sufficiently large value for $x_m (= x_{\max})$ such that the integrand $I(x,y)$ for $x > x_{\max}$ is negligible.

The implementation of this algorithm becomes very simple if the integrand oscillates periodically. Let us first consider the case with $x_0 = 0$ and x_m equal to a multiple of the period P. The number of zeros is given by $N = x_m/P$. The upper and lower limits of the integration segments then become, respectively, $X_i = P$ and $X_{i-1} = (i-1)P$. Numerical tests have shown that when the PGM is applied to an integrand that has either a perfect periodicity (e.g. $\sin x$) or a quasi-periodicity (e.g. $j_n(x)$), the X_i need not be exactly the zeros of the integrand. Consequently, for any given x_0 and properly chosen $x_{\max}$, the algorithm of equation (2) can be implemented with the choice $N = (x_m - x_0)/P$, $X_i = x_0 + (i-1)P$ $(i = 1,2,\ldots,N)$ and $X_{N+1} = x_{\max}$.

It is easy to see that the PGM puts equal emphasis on the integrand between any two successive zeros, no matter how many Gaussian points are used. This feature cannot be easily realized with the 'standard' Gaussian technique where the use of too few points in the interval $[x_0, x_{\max}]$ may result in ignoring the fine structure of the integrand.

3. Numerical examples

The versatility and accuracy of the PGM is demonstrated in this section by considering a familiar example from physics. It is the Fourier transformation, which is also called

the integral Bessel transformation, and is so often encountered in nuclear reactions and structure theories [5,6]. To compare the numerical results with the exact ones, we choose the integrand for which the integration can also be done analytically.

We consider the three-dimensional integral

$$f(q) = \int \mathrm{d}r\, \mathrm{e}^{\mathrm{i}q\cdot r} g(r) \tag{3}$$

where $\mathrm{i} = \sqrt{-1}$. The radial part of the nth multipole decomposition of equation (3) is given by

$$f_n(q) = \int_0^\infty j_n(qr) g(r) r^2 \,\mathrm{d}r \tag{4}$$

where $j_n(qr)$ is the spherical Bessel function of integer order n and $g(r)$ can represent a variety of quantities, e.g. nuclear charge density distribution in nuclear physics [7], spherically averaged one-electron density in atomic physics [8], etc. For $g(r)$ we choose the harmonic oscillator (or Gaussian) function

$$g(r) = r^m \mathrm{e}^{-\alpha^2 r^2} \tag{5}$$

where α is the oscillator constant. The integration in equation (4) can then be done analytically only if $m = n$ or $m = n + 2$. The result is

$$f_n(q) = \begin{cases} 2^{-(n+2)}\sqrt{\pi}\alpha^{-(2n+3)} q^n \mathrm{e}^{-q^2/4\alpha^2} & \text{if } m = n \\ 2^{-(n+2)}\sqrt{\pi}\alpha^{-(2n+5)}(n + 3/2 - q^2/4\alpha^2)\mathrm{e}^{-q^2/4\alpha^2} & \text{if } m = n+2. \end{cases} \tag{6}$$

Numerical evaluation of equation (4) with $g(r)$ given by equation (5) has been carried out for different values of q and different orders ($n = m$) of j_n, using both the 'partitioned' and 'standard' Gaussian methods. The Bessel functions were calculated using Miller's method [9,10]. All calculations were done in double precision on a CDC-7600 computer. The results are compared with the exact ones in tables 1 and 2. For both the PGM and the 'standard' method, the values of α and $r_{\max}$ (upper limit on the integral) are 0.556 fm^{-1} and 16 fm, respectively [6]. As mentioned in section 2, the number of subintervals for the PGM is determined by the number of zeroes in the integrand which, in turn, depends on n and q. Furthermore, the number of Gaussian points for the 'standard' method is taken equal to the number of points per subinterval of the PGM. Thus the PGM uses more points than the 'standard' method. In figure 1 the integrand $r^2 j_n(qr) g(r)$ is shown for $q = 5$ fm^{-1} and $m = n = 5$. For this integrand, the number of subintervals is 9.

The following features are noticeable from the tables. In all cases, the calculations using the PGM converge to the exact results with only one trial requiring 8 points per subinterval. (The total number of points ranges between 72 and 120, depending on the order and argument of the Bessel function.) With the 'standard' Gaussian method, convergence in most of the cases is obtained after four trials requiring at least 64 points. One needs even a larger number of trials as $r_{\max}$ is increased (table 3).

The PGM has also been tested for other forms of $g(r)$ and finite integration limits. One such integral is

$$f_n(a) = \int_0^a \frac{1}{r}\sin(a - r) j_n(r)\,\mathrm{d}r = \frac{a}{[(n + 1/2)^2 - 1/4]} j_n(a) \qquad (n > 0). \tag{7}$$

Table 1. Comparison of the numerical results with the exact ones for $q = 5.0$ fm^{-1} and $r_{max} = 16.0$ fm (upper limit on the integral). n and N_g are, respectively, the order of the Bessel function and number of Gaussian points per subinterval of the PGM. The number of points used for the entire range of the 'standard' method is N_g. The exponent m in equation (5) is equal to n.

n	N_g	'Partitioned'	'Standard'	Exact
5	8	1.60018×10^{-4}	-7.73216×10^{0}	1.60018×10^{-4}
	16	1.60018×10^{-4}	1.32595×10^{1}	
	32	1.60018×10^{-4}	5.84936×10^{-4}	
	64	1.60018×10^{-4}	1.60018×10^{-4}	
25	8	2.04034×10^{14}	-1.43341×10^{15}	2.04034×10^{14}
	16	2.04034×10^{14}	8.26505×10^{14}	
	32	2.04034×10^{14}	2.03626×10^{14}	
	64	2.04034×10^{14}	2.04034×10^{14}	
50	8	8.74222×10^{36}	9.90527×10^{36}	8.74222×10^{36}
	16	8.74222×10^{36}	9.27291×10^{36}	
	32	8.74222×10^{36}	8.74222×10^{36}	

Table 2. The same as table 1 but for $q = 7.5$ fm^{-1}.

n	N_g	'Partitioned'	'Standard'	Exact
25	8	6.30691×10^{7}	-8.17068×10^{14}	6.30691×10^{7}
	16	6.30691×10^{7}	-4.88461×10^{13}	
	32	6.30691×10^{7}	1.08186×10^{13}	
	64	6.30691×10^{7}	6.30691×10^{7}	
50	8	6.82364×10^{34}	-2.08633×10^{37}	6.82364×10^{34}
	16	6.82364×10^{34}	1.48664×10^{37}	
	32	6.82364×10^{34}	1.27468×10^{35}	
	64	6.82364×10^{34}	6.82364×10^{34}	

The results for this equation are identical to those with the harmonic oscillator form for $g(r)$ and are, therefore, not presented here.

It is instructive to examine as to why the 'standard' method requires several trials to make the numerical results stable. This can be done most easily by an inspection of figure 1. From the figure it can be seen that the integrand is negligible between $r = 0$ and $r = 1$ and for $r > 7$. Since in the 'standard' method the Gaussian points are spread in a definite way over the entire range of the integrand $[0, r_{max}]$, a small N_g and large r_{max} tends to pick the integrand where it is negligible and avoid it where it is substantial and has detailed structure (e.g. between $r = 3$ and 4). This kind of problem is avoided in the PGM by forcing the integration between the successive zeros, at the expense of a moderate increase of computing time. For example, for $q = 5$ fm^{-1} and $n = 5$, the total CPU time on a *CDC-7600 computer* taken by the PGM is 0.16 s, as opposed to 0.10 s taken by the 'standard' method. Although the 'standard' method requires less computational time, it is clear that one has to rely to a large extent on intuition or carry out extensive tests to ascertain that the results are meaningful. In most of the calculations the analytic form of $g(r)$ is not known; the application of the 'standard' Gaussian method can then be more problematical. Such extensive tests or intuition are not required if one uses the PGM described in this paper.

Simple but powerful schemes for numerically evaluating integrals of the type given

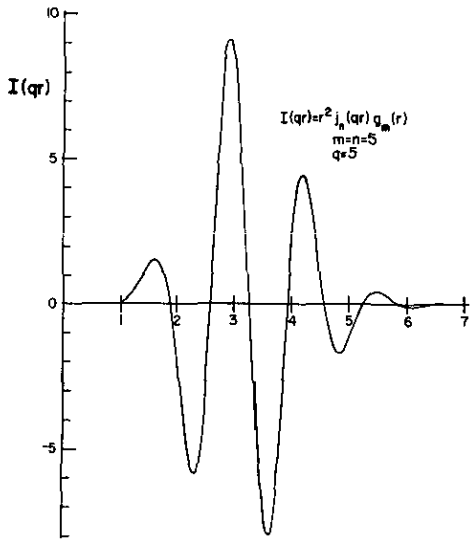

Figure 1. The integrand $j_n(qr)r^{m+2}e^{-\alpha^2 r^2}$ as a function of r.

Table 3. The same as table 1 but for $r_{max} = 32.0$ fm.

n	N_g	'Partitioned'	'Standard'	Exact
5	8	$1.600\,18 \times 10^{-4}$	$2.679\,61 \times 10^{0}$	$1.600\,18 \times 10^{-4}$
	16	$1.600\,18 \times 10^{-4}$	$-8.301\,67 \times 10^{0}$	
	32	$1.600\,18 \times 10^{-4}$	$1.183\,52 \times 10^{0}$	
	64	$1.600\,18 \times 10^{-4}$	$1.602\,29 \times 10^{-4}$	
	80	$1.600\,18 \times 10^{-4}$	$1.600\,18 \times 10^{-4}$	

by equation (4) have also been developed by Sagar *et al* [11], but only for the zeroth-order Bessel function, i.e. $j_0(qr) = \sin(qr)/qr$, which is pertinent for calculations in atomic physics and quantum chemistry. In contrast, the method developed by us is valid for any order of the Bessel function. It is, therefore, useful for nuclear physics calculations also.

We could have performed the integration by partitioning other methods, e.g. Simpsons', trapezoidal, etc, between successive zeroes of the integrand. However, in order to achieve the same numerical accuracy as obtained with the PGM, we would require a very fine mesh size thereby increasing the computational time substantially, in some cases by as much as an order of magnitude. The PGM, therefore, has the advantage that it is faster than the partitioning of other methods mentioned above.

4. Summary and conclusions

In this work a simple but highly accurate method for numerically integrating functions which can have many oscillations has been described. It is a generalization of the 'standard' Gaussian method and reduces to the 'standard' method if the integrand is not oscillatory. The applicability of the method has been tested by considering Fourier

transformation as an example. It is found to yield very good results for substantially large orders and arguments of the Bessel function.

The integrands considered in this work are all analytic and have a convergent Taylor series at each point. The PGM might pose difficulties if the integrands are non-analytic. Further, the method will fail if the integrand has an infinite number of zeros in the interval between 0 and ∞. However, such integrands are seldom encountered in physics or chemistry problems. It should also be mentioned that the convergence rate of the PGM is a little slower than the 'standard' Gaussian method.

The advantage of the PGM is that one does not have to test the numerical convergence integrand by integrand. The use of a small number of Gaussian points for each oscillation segment will ensure convergence to the correct result. This avoidance of the necessity for pre-testing the integration represents a valuable feature of the PGM, especially in the context of a multi-purpose computer code where the integrands are to be supplied, usually in the form of function subprograms, by the users and the oscillatory structure of the integrands cannot be pre-determined once and for all.

Acknowledgment

This work was performed under the auspices of the Division of Nuclear Physics, Office of High Energy and Nuclear Physics, US Department of Energy (Contract No W-7405-ENG-36).

References

[1] Hildebrand F B 1956 *Introduction to Numerical Analysis* (New York: McGraw-Hill)
[2] Dahlquist G, Björck Å and Anderson N 1974 *Numerical Analysis* (Englewood Cliffs, NJ: Prentice-Hall)
[3] Haider Q and Liu L C 1987 Isotope and nuclear chemistry report *Los Alamos National Laboratory Publication* No LA-11034-PR p 187
[4] Erdelyi A (ed) 1954 *Tables of Integral Transforms* vols I and II (New York: McGraw-Hill)
[5] Haider Q and Liu L C 1988 *J. Phys. G: Nucl. Phys.* **14** 1527
[6] Haider Q and Liu L C 1990 *Z. Phys.* A **335** 437
[7] de Jager C W, de Vries H and de Vries C 1974 *At. Data Nucl. Data Tables* **14** 479
[8] Coppens P 1982 *Electron Distributions and Chemical Bonds* ed P Coppens and M B Hall (New York: Plenum)
[9] Abramowitz A and Stegun I A (eds) 1972 *Handbook of Mathematical Functions* (Washington, DC: National Bureau of Standards)
[10] British Association for the Advancement of Science 1950 *Bessel Functions, Part I. Functions of Order Zero and Unity, Mathematical Tables* vol VI (Cambridge: Cambridge University Press)
[11] Sagar R P, Schmider H and Smith Jr V H 1992 *J. Phys. A: Math. Gen.* **25** 189