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A Method for Computing Bessel Function Integrals

M. Puoskari

Department of Theoretical Physics, University of Oulu, Linnanmaa, SF-90570 Oulu 57, Finland

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A method for numerical calculation of integrals containing Bessel functions of integer or integer plus one-half order is described. The calculation involves first a one-dimensional Fourier sine or cosine transform followed by evaluation of the coefficient of the Chebyshev series of the Fourier-transformed function in the case of the Bessel function and evaluation of the Legendre expansion coefficient in the case of the spherical Bessel function. A generalization of the method for the computation of an integral involving the Bessel function of arbitrary real order v is presented as well. \mathbb{C} 1988 Academic Press, Inc.

1. INTRODUCTION

We consider the numerical computation of an integral

$$F_{v}(y) = Ay^{-\mu} \int_{0}^{\infty} x^{\sigma-\mu} f(x) J_{v}(yx) dx, \qquad (1)$$

where $J_{\nu}(yx)$ is the Bessel function of the first kind and of order ν , and ν , y are arbitrary positive real numbers. Special cases of this integral are the Bessel transform (also called the Fourier-Bessel or the Hankel transform) when ν is an integer and $\sigma = 1$, $\mu = 0$, and $A = 2\pi$,

$$F_n(y) = 2\pi \int_0^\infty x f(x) J_n(yx) dx$$
⁽²⁾

and the spherical Bessel transform when v is an integer plus one-half $v = l + \frac{1}{2}$ and $\sigma = 2$, $\mu = \frac{1}{2}$ and $A = 4\pi(\pi/2)^{1/2}$,

$$F_{I}(y) = 4\pi \left(\frac{\pi}{2}\right)^{1/2} \int_{0}^{\infty} x^{2} f(x)(yx)^{-1/2} J_{I+1/2}(yx) dx$$
$$= 4\pi \int_{0}^{\infty} x^{2} f(x) j_{I}(yx) dx,$$
(3)

where $j_i(x)$ is now the spherical Bessel function.

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For the large values of y the integrands of (2) or (3) are rapidly oscillating functions and one must either divide the integral over infinite interval into a sum of integrals over finite intervals between the zeros of the the Bessel functions [1, 2] or use special methods. Several procedures have been described in the literature [3]; one can either approximate the function f(x) by a truncated series of Chebyshev polynomials [4] so that the resulting integrals (so called modified moments of $J_{\nu}(x)$) can be calculated exactly or one can expand it into Laguerre polynomials [5] whose Hankel transforms are known. Other approaches of interest are procedures which are based on the fast Fourier transform (FFT) algorithms: one can replace the argument y and the integration variable x by exponential variables and transform the Bessel integral into a correlation or a convolution integral which can be evaluated by FFT [6, 7] or by some other means [8]. Candel [9] has used the generating function expansion of the Bessel function to convert the integral (2) into two successive Fourier transforms which again can be calculated with FFT. One can also use the projection slice theorem to compute the Hankel transform from the one-dimensional fast Fourier transform of the projection of the function onto the real x-axis [10]. The spherical Bessel function integral (3) was computed by Sommer and Zabolitsky using an extended Filon's integration formula [11].

In this paper we present a method where the integral (1) is transformed to a Fourier sine or cosine transform followed by the integration of the transformed function over the finite interval (-y, y). The weight function of the latter integral is the Chebyshev polynomial in the case of the Bessel integral and the Legendre polynomial in the case of the spherical Bessel integral.

2. Method

At first we calculate the Fourier sine transform if $k = v - \mu$ is odd or the Fourier cosine transform if k is even, where we have to choose v so that k is an integer

$$\widetilde{f}(t) = 2 \int_0^\infty x^\sigma f(x) \sin(tx) \, dx, \quad \text{if} \quad k = v - \mu \text{ is odd}$$

$$\widetilde{f}(t) = 2 \int_0^\infty x^\sigma f(x) \cos(tx) \, dx, \quad \text{if} \quad k = v - \mu \text{ is even.}$$
(4)

Substituting the inverse transforms

$$x^{\sigma}f(x) = \frac{1}{\pi} \int_0^{\infty} \tilde{f}(t) \sin(xt) dt$$

$$x^{\sigma}f(x) = \frac{1}{\pi} \int_0^{\infty} \tilde{f}(t) \cos(xt) dt$$
 (5)

into (1) we obtain

$$F_{\nu}(y) = \frac{Ay^{-\mu}}{\pi} \int_0^\infty \tilde{f}(t) \, \Phi_k(y, t) \, dt \tag{6}$$

when the auxiliary function $\Phi_k(y, t)$ is defined by

$$\Phi_{k}(y,t) = \int_{0}^{\infty} x^{-\mu} J_{2m+1+\mu}(yx) \sin(tx) \, dx, \quad \text{where} \quad k = 2m+1 \text{ is odd,}$$

$$\Phi_{k}(y,t) = \int_{0}^{\infty} x^{-\mu} J_{2m+\mu}(yx) \cos(tx) \, dx, \quad \text{where} \quad k = 2m \text{ is even,}$$
(7)

and *m* is a natural number. These integrals can be calculated in closed form in terms of the Gegenbauer polynomials $C_k^{\mu}(x)$ [12],

$$\Phi_{k}(y, t) = 0, \quad \text{when} \quad t > y$$

$$\Phi_{k}(y, t) = (-1)^{m} (2y)^{\mu - 1} k! \Gamma(\mu)$$

$$\times C_{k}^{\mu}(t/y)(1 - t^{2}/y^{2})^{\mu - 1/2} [\Gamma(k + 2\mu)]^{-1}, \quad \text{when} \quad 0 \le t \le y, \quad (8)$$

where m = (k-1)/2 if k is odd and m = k/2 if k is even.

The Bessel and the spherical Bessel transforms (2) and (3) are then expressed as special cases of (6) using the relations $\mu = 0$, $k = v - \mu = n$, $\lim_{\mu \to 0} \Gamma(\mu) C_k^{\mu}(x) = 2T_k(x)/k$ and $\mu = \frac{1}{2}$, $k = v - \mu = l$, $C_k^{1/2}(x) = P_k(x)$ [13], respectively; the final form of Eq. (2) (*the Bessel integral*) is then

$$F_n(y) = \frac{(-1)^m}{y} \int_{-y}^{y} \tilde{f}(t) (1 - t^2/y^2)^{-1/2} T_n(t/y) dt,$$
(9)

while for Eq. (3) (the spherical Bessel integral) we obtain

$$F_{l}(y) = \frac{(-1)^{m} \pi}{y} \int_{-y}^{y} \tilde{f}(t) P_{l}(t/y) dt, \qquad (10)$$

where T_n is the Chebyshev polynomial and P_l is the Legendre polynomial.

Linz [14] earlier derived the result of Eq. (9) for the Bessel function $J_0(x)$ by means of an Abel transform. In this case the integral (9) is simply

$$F_{n=0} = 2 \int_0^y (y^2 - t^2)^{-1/2} \left[2 \int_0^\infty x f(x) \cos(tx) \, dx \right] dt. \tag{11}$$

Also, Mook recently used the Abel transform to calculate the zeroth order Hankel

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transform [15]. The change of the variable $t = y \cos \theta$ in Eq. (9) yields an equation which is quite similar to that used by Candel for the Bessel transform [9],

$$F_n(y) = (-1)^m \int_0^\pi \tilde{f}(y\cos\theta)\cos(n\theta) \,d\theta.$$
(12)

In addition, we note that the formulas related to Eqs. (9) and (10) are discussed in Section 3.2 of the survey of the Bessel function integrals by Piessens and Branders [3].

The calculation of the Bessel integrals is thus reduced to computation of the Chebyshev series coefficient or to computation of the Legendre expansion coefficient of the one-dimensional Fourier transform of f(x). The Fourier transforms can be calculated using either FFT [16] or the adaptive procedure of Piessens and Branders [1, 17] by introducing the upper limit cutoff X_{max} in the infinite range integrals (4). We have used the latter approach since then one can choose the abscissae of $\tilde{f}(t)$, whereas if FFT is used one has to interpolate to obtain the values of $\tilde{f}(t)$ on the Chebyshev abscissae $t_j = \cos(j\pi/N)$ in Clenshaw–Curtis rules or if one uses adaptive integration routines to calculate integrals (9) and (10). In the present paper we have employed the NAG routine D01ANF [18] which is based on the QUADPACK routine QAWF of Piessens *et al.* [1]. If the FFT is used the computation of the integral (9) can be made with the algorithm presented by Candel [9].

The Chebyshev coefficient can be calculated by the QUADPACK routine QAWS or by the equivalent NAG routine D01APF while the Legendre coefficient can be calculated using any integrator appropriate to smooth functions, e.g., either QNS or QAG of QUADPACK or either D01AJF or D01AHF of NAG. Another possibility to calculate the Chebyshev series coefficients is to use the recurrence relations due to Clenshaw [19, 20] and we have have used the NAG routine E02AFF which is a modification of this algorithm. Piessens [21] has developed an algorithm (LEGSER, Algorithm 473 of CACM) for calculation of the Legendre expansion coefficient when the Chebyshev series coefficients of the function are known.

3. NUMERICAL EXAMPLES

We have tested our method using some commonly used integrals found in literature on the subject [4, 9, 22, 23]. In the case of the Bessel transform we consider integrals

$$I_{1}(y) = \int_{0}^{\infty} e^{-2x} J_{n}(yx) dx$$

= $y^{-n} [(4 + y^{2})^{1/2} - 2]^{n} (4 + y^{2})^{-1/2}$ (13)

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$$I_{2}(y) = \int_{0}^{\infty} x \frac{\sin(bx)}{(bx)^{2}} J_{n}(yx) dx$$

= $\frac{1}{b^{2}n} \frac{(y/b)^{n} \sin(n\pi/2)}{[1 + (1 - y^{2}/b^{2})^{1/2}]^{n}}, \quad \text{for } 0 \le y \le b$
= $\frac{1}{b^{2}n} \sin[n \arcsin(b/y)], \quad \text{for } y \ge b.$ (14)

The first integral was used by Piessens and Branders [4] to test their Bessel function integrator bases on the Chebyshev series expansion of f(x) and the second one is a special case of the Weber-Schafheitlin integral and was used by Candel [9] in his FFT calculations.

In the case of the spherical Bessel transform we compute the integral

$$I_{3} = \int_{0}^{\infty} x^{l+2} e^{-ax} j_{l}(yx) dx$$

= $2^{l+1}(l+1)! ay^{l}(a^{2}+y^{2})^{-(l+2)}$ (15)

which was also used as a test integral by Talman [7, 23] and by Sommer and Zabolitsky [11].

The Fourier integrals are computed using the automatic Fourier integrator D01ANF of the NAG library with requested relative accuracy EPSREL (which was in our calculation typically 10^{-4} or 10^{-3}). The integrals in (9) and (10) have been evaluated with two different methods: the Chebyshev coefficients or the Legendre series coefficients were computed either by a recurrence relation method of Clenshaw or by direct numerical integration methods. We calculated the Chebyshev coefficients using the NAG routine E02AFF. The same routine was employed to calculate the Chebyshev coefficients of $\tilde{f}(t)$ in (10) whereafter the Legendre series coefficients were computed by the routine LEGSER of Piessens [21]. The integrals (9) and (10) were also computed by the adaptive NAG routines D01APF and D01AHF, respectively, with the requested relative accuracy of 10^{-4} for D01AHF and 10^{-3} for D01APF.

The resume of the integration routines and input parameters which are actually needed in the present computation is presented in Table I. The input parameters in the adaptive integration method were the upper limit of the Fourier integral XMAX and the requested relative accuracy EPSREL in the NAG integration routines. In the recurrence relation method the additional input parameter was the number of the points N, where the Fourier integral $\tilde{f}(t)$ has to be calculated, which is equivalent to the number of Chebyshev coefficients used in the NAG routine E02AFF.

The computations were carried out on VAX11/730 and on IBM3083 using double precision arithmetic. The absolute errors of the numerical integration together with the exact values of the integrals are presented in Talbe II for the

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TABLE I

Combinations of NAG Routines Which Were Used in Evaluation of the Bessel Integrals I_1 and I_2 and the Spherical Bessel Integral I_3 with the Recurrence Relation Method (Method 1) or with the Adaptive Numerical Integration Method (Method 2) and the Input Parameters Which Are Needed in the Integration Routines

	Method 1	Method 2
Calculation of the Fourier integral (4)	D01ANF	D01ANF
Calculation of the Bessel integral (9)	E02AFF	D01APF
Calculation of the spherical Bessel integral (10)	E02AFF + LEGSER	D01AHF
Input parameters	EPSREL = the required relative accuracy XMAX = the upper limit of the Fourier integral N = the number of points where the Fourier integral is calculated	EPSREL = the required relative accuracy XMAX = the upper limit of the Fourier integral

TABLE II

Integral I_1 (13)) Calculated with	XMAX = 30
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п	y	Exact integral	Method 1 Absolute error	Method 2 Absolute error
0	1	0.44721360	0.954×10^{-12}	-0.790×10^{-11}
	10	$0.98058068 \times 10^{-1}$	0.541×10^{-13}	-0.756×10^{-11}
	100	$0.99980006 \times 10^{-2}$	0.676×10^{-14}	0.367×10^{-5}
	1000	$0.99999800 \times 10^{-3}$	0.673×10^{-6}	$0.620 \times 10^{-3} a$
5	10	$0.36310584 \times 10^{-1}$	-0.729×10^{-14}	0.923×10^{-11}
	100	$0.90466253 \times 10^{-2}$	0.752×10^{-13}	-0.406×10^{-6}
	1000	$0.99004786 \times 10^{-3}$	-0.673×10^{-8}	-0.127×10^{-5}
10	1	$0.24037306 \times 10^{-6}$	-0.326×10^{-12}	0.364×10^{-12}
	10	$0.13445692 \times 10^{-1}$	0.489×10^{-13}	-0.291×10^{-10}
	100	$0.81857797 \times 10^{-2}$	0.676×10^{-14}	$0.367 \times 10^{-5 a}$
	1000	$0.98019673 \times 10^{-3}$	-0.673×10^{-6}	0.689×10^{-3} °

^a The requested tolerance in the D01APF integration routine was not achieved due to a bad local integrand behavior.

Note. In the recurrence relation method (Method 1) EPSREL = 10^{-4} and N = 250 for y = 1, 10 and N = 2000 for y = 100, 1000, while in the adaptive numerical integration method (Method 2) EPSREL = 10^{-3} for y = 1, 10, and 10^{-2} for y = 100, 1000, and for all values of y in the case of n = 10.

TABLE	III

n	у	Exact integral	Method 1 Absolute error	Method 2 Absolute error
0	0.1	0.24875462	-0.104×10^{-16}	-0.693×10^{-17}
	1	0.16000000	0.201×10^{-15}	0.298×10^{-15}
	5	$0.47562426 \times 10^{-2}$	0.285×10^{-16}	0.144×10^{-7}
	10	$0.36982246 \times 10^{-3}$	0.210×10^{-16}	-0.764×10^{-10}
	20	$0.24507401 \times 10^{-4}$	-0.236×10^{-17}	0.103×10^{-16}
	50	0.63795690 × 10 ⁻⁶	0.221×10^{-16}	0.122×10^{-12}
	100	$0.39968019 \times 10^{-7}$	0.963×10^{-17}	0.760×10^{-13}
5	0.1	$0.55275395 \times 10^{-4}$	-0.608×10^{-16}	-0.311×10^{-16}
	1	$0.11796480 \times 10^{+1}$	-0.501×10^{-10}	-0.815×10^{-7}
	5	$0.16695772 \times 10^{-1}$	-0.814×10^{-12}	0.420×10^{-8}
	10	$0.70034026 \times 10^{-4}$	-0.196×10^{-12}	-0.262×10^{-12}
	20	$0.16788925 \times 10^{-6}$	-0.921×10^{-11}	0.652×10^{-11}
	50	$0.46660804 \times 10^{-10}$	0.324×10^{-13}	0.368×10^{-13}
	100	$0.91902364 \times 10^{-13}$	-0.466×10^{-11} a	$0.343 \times 10^{-13 a}$

Integral I_3	(15)) Calculated	with	XMAX = 40	and	a = 2
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^a Roundoff errors in the D01ANF routine prevented the requested tolerance from being achieved.

Note. In the recurrence relation method (Method 1) EPSREL = 10^{-4} and N = 250 for $y \le 20$ and N = 1000 for y = 50, 100, while in the adaptive numerical integration method (Method 2) EPSREL = 10^{-4} .

Bessel function integral I_1 (13) and in Table III for the spherical Bessel function integral I_3 (15). In Fig. 1 the result for the integral I_2 (14) are compared with the exact values of that integral.

The results from the Clenshaw recurrence relation method are accurate to more than 10 decimal places for the smooth integrals (13) and (15) except for the very large values of y in the Bessel integral (13), where the accuracy was about 6-8decimal places. The results from the direct integrations of the Chebyshev and the Legendre series coefficients are accurate to about 7-8 decimal places in most cases. The routine D01AHF which is based on the optionally extended Gauss rules in an adaptive strategy due to Patterson [24] turned out to be faster than the routine D01AJF in computation of the Legendre series coefficient (10). We found that the routine D01APF failed in calculation of the Chebyshev coefficient for large values of y. The accuracy of the integral I_2 (14) (which is about 5 decimal places) is limited by the upper limit cutoff of the Fourier integral XMAX = 150, where the value of the integrand is about the same order as the obtained absolute error of the calculation. The accuracy of the results of the integral I_2 were yet two decades poorer at y = b where the first derivative of the integral is discontinuous. In the scale of Fig. 1 our results for I_2 are similar to Candel's FFT calculations [9], except for the case of l=7 when $y \approx b = 0.2$, where our estimates seem to be inferior to those of Candel.



FIG. 1. The Bessel integral I_2 (14) for b = 0.2. The exact integrals are represented as solid lines. Estimates from numerical computations with the recurrence relation method (Method 1) are represented by dots (\cdot). The input parameters are XMAX = 150, N = 500, and EPSREL = 10^{-4} : (A) l = 0; (B) l = 1; (C) l = 7.

4. A GENERALIZATION

Lastly we present a numerical calculation of the general Bessel integral (1). Expressing Gegenbauer polynomials in terms of the hypergeometric function $2F_1$ [13],

$$C_{k}^{\mu}(x) = \frac{\Gamma(k+\mu)}{k! \, \Gamma(2\mu)} \, 2F_{1}\left(k+2\mu, -k; \, \mu+\frac{1}{2}; \frac{1-x}{2}\right),\tag{16}$$

we obtain from Eqs. (6) and (8) for the Bessel integral,

$$F_{\nu}(y) = \frac{Ay^{-2y}}{2\pi} \frac{2^{\mu-1} \Gamma(\mu)}{\Gamma(2\mu)} (-1)^m \int_{-y}^{y} \tilde{f}(t) (y^2 - t^2)^{\mu-1/2} \times {}_2F_1\left(k + 2\mu, -k; \mu + \frac{1}{2}; \frac{1 - t/y}{2}\right),$$
(17)

where m = (k-1)/2 when k is odd and m = k/2 when k is even.

To test Eq. (17) we evaluate the integral

$$I_{4}(y) = \int_{0}^{\infty} x^{\beta - 1} e^{-ax} J_{\nu}(yx) dx$$

= $\frac{y}{2a} \frac{\nu \Gamma(\beta + \nu)}{a^{\beta} \Gamma(\nu + 1)} {}_{2}F_{1}\left(\frac{\nu + \beta}{2}, \frac{\nu + \beta + 1}{2}; \nu + 1; \frac{-y^{2}}{a^{2}}\right).$ (18)

This integral reduces to the integral (1) when we choose $A = y^{\mu}$, and $\beta = \sigma + 1 - \mu$. The parameter μ has to be chosen so that $k = v - \mu$ is an integer and preferably also $\mu \ge \frac{1}{2}$ to avoid the end-point singularities in Eq. (17). The results for several values of v, β , and y are given in Table IV. The Fourier integrals were again calculated by the NAG routine D01ANF and the integral (17) was computed using the routine D01AHF with a requested relative accuracy of 10^{-4} . The hypergeometric function

v	β	σ	μ	y	Exact integral	Absolute error
1	0	0	0	1	0.23606798	-0.296×10^{-8}
				10	0.81980390	0.142×10^{-5}
				100	0.98019998	0.113×10^{-5}
10	0	0	1	1	$0.53749050 \times 10^{-7}$	-0.136×10^{-10}
				100	$0.81874167 \times 10^{-1}$	-0.262×10^{-6}
0.5	2.5	2	0.5	10	$0.93311117 \times 10^{-3}$	-0.158×10^{-9}
				100	$0.31557004 \times 10^{-6}$	-0.333×10^{-8}
1.5	2.5	2	0.5	1	$0.63830767 \times 10^{-1}$	0.237×10^{-8}
				100	$0.15944926 \times 10^{-4}$	-0.672×10^{-11}
10.5	2.5	2	0.5	10	$0.13132359 \times 10^{-1}$	-0.348×10^{-10}
				100	$0.27586445 \times 10^{-3}$	0.203×10^{-11}
1.25	1.75	2	1.25	10	$0.17833078 \times 10^{-1}$	0.565×10^{-9}
				100	$0.37863949 \times 10^{-3}$	-0.161×10^{-8}
0.75	2.25	2	0.75	10	$0.18978529 \times 10^{-2}$	-0.270×10^{-7}
4.75	2.25	2	0.75	1	0.15316299 × 10 ⁻⁴	0.115×10^{-8}
				100	$0.20172978 \times 10^{-2}$	0.841×10^{-8}

TABLE IV Integral L (18) Calculated with XMAX = 30 and a = 2

Note. The adaptive numerical integration routine D01AHF is used with EPSREL = 10^{-4} .

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 $_{2}F_{1}$ is computed using the algorithm R2F1 presented by Luke [25] for the rational approximation of $_{2}F_{1}(a, b; c; -z)$. The accuracy of the results is seen to be at least 6 decimal places in most cases and usually even more.

5. CONCLUSIONS

We have presented a new method for the computation of integrals of the form (2) or (3). The method can be generalized also for calculation of the general Bessel function integral (1) even if v is not an integer or an integer plus one-half.

The adaptive integration procedure converged rather slowly when the argument y is large (especially in the case of the Bessel integral). The recurrence relation method of Clenshaw in the calculation of the Chebyshev coefficient (9) is faster but for larger values of the argument y also, this method requires computation of a rather larger number of points of the Fourier transform f(t). It has, however, the advantage that all odd (or even) order transforms can be calculated simultaneously.

If one wants to compute the integrals efficiently for many values of the argument y simultaneously it is probably better to construct an algorithm which employs FFT in computation of the Fourier transforms as well as of the Chebyshev coefficient, rather than using the present library routines.

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