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ON NUMERICAL EVALUATION OF INTEGRALS INVOLVING BESSEL FUNCTIONS

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Summary. The paper is concerned with the efficient evaluation of the integral $\int_0^{\infty} f(x) J_n(rx) dx$, where J_n is the Bessel function of index *n* and *n* is a nonnegative integer, for a given sequence of values of a real parameter *r*.

Two procedures are proposed and compared. One of them consists in a direct generalization of a procedure for the evaluation of a similar integral with the weight function $\exp(irx)$, which employs the fast Fourier transform. The other approach is based on the construction of a special Gaussian quadrature formula where J_n appears as a weight.

The results of the comparison show that the application of the Gaussian formula is much more efficient.

Keywords: integrals involving Bessel functions, numerical quadrature, fast Fourier transform, Gaussian quadrature formula.

AMS Classification: 65D32.

1. INTRODUCTION

The paper is concerned with the efficient evaluation of the integral

(1.1)
$$\int_0^\infty f(x) J_n(rx) dx$$

where J_n is the Bessel function of index *n* (*n* being a nonnegative integer).

A similar problem to evaluate the integral

(1.2)
$$\int_{0}^{\infty} f(x) \exp(irx) dx, \quad r = r_0, ..., r_j$$

or the integrals

$$\int_0^\infty f(x) \cos rx \, \mathrm{d}x \quad \text{and} \quad \int_0^\infty f(x) \sin rx \, \mathrm{d}x \; ,$$

is often met in computational practice. For example, the computation of the quantities of electromagnetic field in the homogeneous or layered Earth at depth r in the presence of a harmonic line source can be performed as the evaluation of (1.2) with

a particular decreasing function f [4]. Many numerical procedures for the solution of this problem have been proposed and analysed (see e.g. [6], [8], [13], [14], [17]). The procedure described by Bezvoda and Segeth [5] is based on the employment of the trapezoidal rule (on a finite interval (0, L)), which is evaluated with the help of the fast Fourier transform (FFT) and yields simultaneously the values of (1.2) for

$$r_i = 2\pi j | (Nh), \quad j = 0, ..., N/2.$$

Here, h is the integration step, $N = 2^{\nu}$ (ν is a positive integer), and L = (N - 1) h. The fast Fourier transform then operates on N values and the total number of arithmetic operations required for the simultaneous calculation of (1.2) is $O(N \log N)$.

Various problems in geophysics, for example the computation of the quantities of electromagnetic field at depth r in the presence of a harmonic point source, are reduced to the evaluation of the integral (1.1) for $r = r_0, ..., r_J$ [7]. Apparently, this problem, which we are going to discuss in the paper, is more complex than the previous one. We follow a natural generalization of the above described procedure for the simultaneous computation of the integral (1.2) (see e.g. [1]) and show that the construction and application of a Gaussian quadrature formula (where J_n appears as a weight) is more efficient.

2. THE TRAPEZOIDAL FORMULA WITH A FFT COMPUTATION OF J_n

The problem whose solution we discuss in this paper is the evaluation of the integral

(2.1)
$$I_n(r) = \int_0^\infty f(x) J_n(rx) dx$$

for a given set of values of the real parameter $r, r = r_0, ..., r_J$. Further, J_n is the Bessel function of index n, n being a nonnegative integer, and f is a complex-valued Lebesgue-integrable function defined on $(0, +\infty)$.

Choosing an integration step h_1 and a positive integer N_1 , we may replace the `integral $I_n(r)$ by its trapezoidal formula approximation,

(2.2)
$$I_n(r) \approx I_n^*(r) = h_1(\frac{1}{2}f(0) J_n(0) + \sum_{p=1}^{N_1-2} f(ph_1) J_n(rph_1) + \frac{1}{2}f(L_1) J_n(rL_1)),$$

where $L_1 = (N_1 - 1) h_1$ is the length of the interval of actual numerical integration.

If we now calculate $I_n^*(r)$ and take this value for the approximation to $I_n(r)$, the error of this approximation consists of three components. First, we replace the infinite upper limit of integration by a finite number L_1 . A discussion of the influence of the choice of L_1 on the error of the integration is the subject of e.g. Gustafson and Dahlquist [10]. This error is usually of little importance in practical computation since in most cases f(x) decreases rapidly as $x \to \infty$.

Second,

$$\int_{0}^{L_{1}} f(x) J_{n}(rx) dx - I_{n}^{*}(r) = R_{1},$$

where

(2.3)
$$R_1 = -\frac{1}{12}L_1h_1^2(f(\xi) \mathbf{J}_n(r\xi))^n, \quad \xi \in (0, L_1),$$

is the error of the trapezoidal formula [15]. Finally, the roundoff error contributes to the total error, too, but its influence is very weak [15].

Any numerical procedure for the computation of (2.1) has to perform the evaluation of the Bessel function J_n at some (perhaps many) points. A way of a simultaneous computation of the values $J_n(rx)$, $r = r_0, r_1, ..., r_J$, for a fixed x > 0 follows from the integral representation ([9], formula 8.411.7)

$$\mathbf{J}_n(x) = \frac{\left(\frac{x}{2}\right)^n}{\Gamma(n+\frac{1}{2})\,\Gamma(\frac{1}{2})} \int_0^n \exp\left(\mathrm{i}x\,\cos t\right)\sin^{2n}t\,\mathrm{d}t\,,$$

where Γ is the gamma function. The substitution $y = x \cos t$ yields

(2.4)
$$J_n(rx) = \frac{\left(\frac{r}{2x}\right)^n}{\Gamma(n+\frac{1}{2})\,\Gamma(\frac{1}{2})} \int_{-x}^x (x^2 - y^2)^{n-1/2} \exp\left(iry\right) dy \,.$$

Putting

$$g_{n,x}(y) = (x^2 - y^2)^{n-1/2} \text{ for } |y| \le x,$$

= 0 elsewhere,

we can write

(2.5)
$$J_n(rx) = \frac{\left(\frac{r}{2x}\right)^n}{\Gamma(n+\frac{1}{2})\Gamma(\frac{1}{2})} \int_{-\infty}^{\infty} g_{n,x}(y) \exp(iry) \, \mathrm{d}y \, ,$$

i.e., the Bessel function $J_n(rx)$ is the Fourier transform of the function $g_{n,x}(y)$ (apart from a multiplicative constant). We now consider x to be a parameter.

As we have to evaluate $J_n(rx)$ for $x = h_1, 2h_1, ..., (N_1 - 1) h_1$ (cf. (2.2)) and a sequence of parameters $r = r_j$, we choose

$$(2.6) L_2 \ge L_1$$

and apply to (2.5) the trapezoidal formula with an integration step h_2 and a positive integer N_2 such that $L_2 = (N_2 - 1) h_2$. We obtain

(2.7)
$$J_n(rx) \approx \frac{\left(\frac{r}{2x}\right)^n}{\Gamma(n+\frac{1}{2})\,\Gamma(\frac{1}{2})} h_2(\frac{1}{2}g_{n,x}(-L_2)\exp\left(-irL_2\right) +$$

$$+\sum_{k=-N_{2}+2}^{N_{2}-2} g_{n,x}(kh_{2}) \exp(irkh_{2}) + \frac{1}{2}g_{n,x}(L_{2}) \exp(irL_{2})) =$$

$$= \frac{\left(\frac{r}{2x}\right)^{n}}{\Gamma(n+\frac{1}{2})\Gamma(\frac{1}{2})} h_{2}(\frac{1}{2}g_{n,x}(0) + \sum_{k=1}^{N_{2}-2} g_{n,x}(kh_{2}) \exp(-irkh_{2}) +$$

$$+ \frac{1}{2}g_{n,x}(L_{2}) \exp(-irL_{2}) + \frac{1}{2}g_{n,x}(0) +$$

$$+ \sum_{k=1}^{N_{2}-2} g_{n,x}(kh_{2}) \exp(irkh_{2}) + \frac{1}{2}g_{n,x}(L_{2}) \exp(irL_{2}))$$

as the function $g_{n,x}$ is even. Note that the condition (2.6) guarantees that the function $g_{n,x}$ is always numerically integrated in (2.7) over its whole support. Therefore, the error involved in the replacement of $J_n(rx)$ by the formula (2.7) has only two components. The error of the trapezoidal rule, similarly to (2.3), is given [15] by

(2.8)
$$R_{2} = -\frac{1}{6}L_{2}h_{2}^{2} \frac{\left(\frac{r}{2x}\right)^{n}}{\Gamma(n+\frac{1}{2})\Gamma(\frac{1}{2})} (g_{n,x}(\eta)\exp(ir\eta))^{n}, \eta \in (-L_{2},L_{2}),$$

while the roundoff error is again negligible.

The formula in (2.7) can be evaluated for a fixed x and simultaneously for all $r = r_j$ if we put

(2.9)
$$r_j = 2\pi j / (N_2 h_2), \quad j = 0, ..., N_2 / 2, \quad N_2 = 2^{\nu_2}$$

with a positive integer v_2 and use the fast Fourier transform. Denoting by

$$\gamma_{n,x} = (\frac{1}{2}g_{n,x}(0), g_{n,x}(h_2), \dots, g_{n,x}(N_2 - 2) h_2), \frac{1}{2}g_{n,x}(L_2))$$

a vector having N_2 components and by $\beta_{n,x} = ((b_{n,x})_j)$ its discrete Fourier transform (having also N_2 components), we arrive at

(2.10)
$$\mathbf{J}_{n}(r_{j}x) \approx \frac{\left(\frac{r_{j}}{2x}\right)^{n}}{\Gamma(n+\frac{1}{2})\,\Gamma(\frac{1}{2})}\,h_{2}((b_{n,x})_{j}+(b_{n,x})_{N_{2}-j})$$

with r_i given in (2.9) since

$$\exp\left(-2\pi i j k/N_2\right) = \exp\left(2\pi i (N_2 - j) k/N_2\right).$$

The employment of the fast Fourier transform for the numerical evaluation of (2.7) may cause an increase of the roundoff error as compared with the direct computation (see e.g. [11], [16]). This feature, however, did not show significant in practical computation.

Note that we cannot obtain the value of $J_n(0)$ in this way. However, we have $J_0(0) = 1$ and $J_n(0) = 0$ for n > 0 (see e.g. [9]).

A problem arises in case of n = 0 as $g_{0,x}(y)$ has a singularity for y = x. We will turn back to the case of n = 0 later. For n > 0, we have $g_{n,x}(x) = 0$. Unfortunately, for $n \leq 2$ the second derivative $g''_{n,x}$, which appears in (2.8), has also a singularity at y = x and it is thus rather hard to obtain a reliable estimate for the error R_2 .

Let us review the algorithm for the evaluation of the integral (2.1) for n > 0. Choose h_1, N_1 (cf. (2.2)) and $h_2, N_2 = 2^{v_2}$ (cf. (2.7), (2.9)). For a fixed $x = ph_1$, (2.10) is evaluated simultaneously for all r_j given by (2.9). This evaluation consists of the determination of the components of the vector γ_{n,ph_1} , the computation of its discrete Fourier transform β_{n,ph_1} , and the substitution into to the formula (2.10), where $x = ph_1$. This is repeated successively for $x = ph_1$, $p = 1, ..., N_1 - 1$, and the values of $J_n(r_jph_1)$ obtained are summed up with weights $f(ph_1)$ in accord with (2.2).

Apparently, the evaluation of (2.10) based on the fast Fourier transform of a vector having N_2 components requires $O(N_2 \log N_2)$ arithmetic operations for a fixed x and is repeated $(N_1 - 1)$ times. Thus the total number of arithmetic operations for the evaluation of (2.2) is $O(N_1N_2 \log N_2)$.

The procedure presented is closely connected with the two-dimensional Fourier transform. Introducing an "artificial" parameter w and taking (2.1) into account, we put

(2.11)
$$\hat{I}_n(r,w) = \int_{-\infty}^{\infty} f(x) J_n(rx) \exp(iwx) dx.$$

For any function f such that $f(x) \equiv 0$ for x < 0, we have

(2.12)
$$I_n(r) = \hat{I}_n(r, 0)$$
.

Obviously, (2.11) is the Fourier transform of the function $f(x) J_n(rx)$ from (2.1) prolonged in an apparent way into $(-\infty, +\infty)$. Now, substituting (2.5) for $J_n(rx)$ into (2.11), we find out that $\hat{I}_n(r, w)$ is the two-dimensional Fourier transform of the function $f(x) g_{n,x}(y)$ but, with respect to (2.12), we are interested only in the value of this transform for fixed w = 0.

The formula (2.2) with the evaluation of $J_n(r_j x)$ by (2.10) is the discrete analog of the idea just formulated continuously. Another computer implementation different from that presented above is also possible. We can approximate $\hat{I}_n(r, w)$, the twodimensional Fourier transform of $f(x) g_{n,x}(y)$, by the discrete Fourier transform, evaluate the latter by the two-dimensional $(N_1 \times N_2)$ fast Fourier transform and keep only those N_2 values of the result which correspond to w = 0. This procedure requires $O(N_1N_2 \log N_1 \log N_2)$ operations, which is (in order) only slightly more than the previous one, but it is always still slower than this previous procedure.

Finally, we mention briefly the evaluation of $I_0(r)$. For the reason that we have discussed above, it is advantageous to integrate by parts in (2.4) to obtain

$$J_0(rx) = \frac{2}{\Gamma^2(\frac{1}{2})} \left(\frac{1}{2}\pi - r \int_0^x \arccos(y/x) \sin(ry) \, dy \right).$$

We can thus use the formula (2.2) for the evaluation of $I_0(r)$, too. Only the formula (2.7) (and, consequently, also (2.10)) is to be changed in a proper way (including a different definition of the function $g_{0,x}$).

3. THE GAUSSIAN FORMULA WITH J_n AS A WEIGHT

The Gauss quadrature formula is well-known and has been studied for a long time. Using this idea, we can obtain quadratures which employ m abscissae and are exact for polynomials of degree 2m - 1.

In literature one can often read that if a function F(x) cannot be well approximated by polynomials but the function f(x) = F(x)/p(x) is well approximated by polynomials (for example, if F(x) is a product of a high-frequency oscillation function and a slowly varying one) and, moreover, if p(x) can be simply integrated, then it is advisable (see e.g. [2]) to use the Gaussian quadrature with the weight function p(x),

(3.1)
$$\int_{a}^{b} p(x) f(x) dx \approx \sum_{j=1}^{m} c_j f(x_j),$$

where the c_j 's naturally depend on p(x). In the literature one can find the tables of x_j and c_j for functions $p(x) \equiv 1$, $p(x) = (1 - x^2)^{-1/2}$ (which is connected with the approximation by Chebyshev polynomials), $p(x) = \cos x$, and some others as well as ready-to-use subroutines (see e.g. [14]).

However, the number of applications of the Gaussian quadrature is very small though the possibility to use the quadrature of higher order accuracy should have been inviting. The main reason probably is that it is difficult to solve the problem of determining x_j and c_j for an arbitrary p(x). For

$$(3.2) p(x) \ge 0,$$

the algorithm is simple [3], but the condition (3.2) is rather disagreeable. In addition, it is necessary to suppose that the moments

(3.3)
$$\mu_k = \int_a^b x^k \, p(x) \, \mathrm{d}x \,, \quad k = 0, 1, \dots,$$

can be exactly evaluated.

The employment of the Gaussian formula to calculate (2.1) demonstrates a possibility to use this quadrature for other purposes. Now the Bessel functions have been chosen as weight functions not for the reason that computing the integrals (3.3) is simple. Quite to the contrary, the difficulty in computing the Bessel functions (more precisely, the long computing time needed) suggests us to construct the quadrature (3.1), as the evaluation of f(x) is simpler than the evaluation of p'(x). For instance in geophysics it is necessary to compute very many integrals of type (2.1) with varying complex functions f(x). In this case it is advisable to determine (once for all) the abscissae x_i and the coefficients c_i and to use them for every f(x).

Now let us deal with the approximate evaluation of the integral (2.1). We first perform a substitution and, as usual, replace the infinite interval by a finite one:

(3.4)
$$I_n(r) \approx \int_0^{z_N} \mathbf{J}_n(z) f\left(\frac{z}{r}\right) \frac{\mathrm{d}z}{r} = \int_0^{z_N} \mathbf{J}_n(z) \tilde{f}(z) \,\mathrm{d}z$$

Further, the interval $(0, z_N)$ is divided by the positive roots of $J_n(z)$ denoted by z_i , i = 1, ..., N; in addition, we put $z_0 = 0$. In every interval $l_i = (z_{i-1}, z_i)$ the condition (3.2) is thus easily satisfied. (For the sake of simplicity, we do not indicate the apparent dependence of z_i and l_i on the parameter n.) After that in every interval l_i the abscissae x_j and coefficients c_j (j = 1, ..., m) are determined. (Their dependence on n and i is not indicated, either.)

Let us shortly describe the algorithm for determining x_j and c_j in a general interval $l_i = (a, b)$.

The set of polynomials orthogonal with the weight p'_{x} ,

(3.5)
$$Q_k(x) = \sum_{j=1}^{k} q_j^{(k)} x^j, \quad q_k^{(k)} = 1, \quad k = 0, 1, \dots,$$

can be constructed by the recurrent formulae

(3.6)
$$Q_0 = 1,$$
$$Q_1 = x - \mu_1 / \mu_0,$$
$$Q_k = (x - \alpha_k^{(1)}) Q_{k-1} - \alpha_k^{(2)} Q_{k-2}, \quad k = 2, ...,$$

where

(3.7)
$$\alpha_{k}^{(1)} = \frac{\int_{a}^{b} p(x) x Q_{k-1}^{2} dx}{\int_{a}^{b} p(x) Q_{k-1}^{2} dx}, \quad \alpha_{k}^{(2)} = \frac{\int_{a}^{b} p(x) x Q_{k-1} Q_{k-2} dx}{\int_{a}^{b} p(x) Q_{k-2}^{2} dx}$$

The coefficients $\alpha_k^{(1)}$ and $\alpha_k^{(2)}$ can be found using the moments μ_i (3.3). For Q_k , we need μ_i , i = 0, 1, ..., 2k - 1.

It is known [3] that x_j are the roots of the polynomial $\omega_m(x)$ of degree m which is orthogonal with weight to all polynomials P_k of degree $k \leq m - 1$. Since P_k may be expressed as a linear combination

$$P_k(x) = \sum_{i=0}^k d_i Q_i(x), \quad k \le m - 1,$$

and Q_i form a system of orthogonal polynomials we have

$$\omega_m(x) = Q_m(x)$$

and thus the x_j 's are the roots of the polynomial Q_m which we obtain from (3.6) and (3.7) if we put $p(x) = J_n(x)$. It has been proved [3], [12] that all the roots lie inside the interval $l_i = (a, b)$ and that all $c_j > 0$.

As soon as the abscissae x_j are determined the coefficients c_j may be computed e.g. from the linear system

(3.8)
$$\sum_{j=1}^{m} c_j x_j^k = \mu_k, \quad k = 0, 1, ..., m-1$$

There is also an explicit formula for the coefficients c_i [12],

$$c_j = \frac{1}{Q'_n(x_j) Q_{n-1}(x_j)},$$

but it is not well suited for the evaluation.

All the above procedures assume $p(x) \ge 0$, which is true in intervals l_i with odd indices. If the index *i* is even we put

$$\mu_k = \int_{z_{i-1}}^{z_i} x^k \big| \mathbf{J}_n(x) \big| \, \mathrm{d}x$$

and the coefficients c_j determined from (3.8) are used in these intervals with an inverse sign.

The moments (3.3) have been computed in double precision by the Simpson formula with 40 subintervals in each l_i . Special measures, including proper substitutions, have been taken in order that these integrals be evaluated very precisely. The use of five abscissae x_j (m = 5) means that the function $\tilde{f}(z)$ in (3.4) is approximated in every interval l_i by a polynomial of degree 9. The abscissae x_j and the coefficients c_j have been determined for $J_n(z)$, n = 0, 1, and for 14 intervals (N = 14). The values of x_j and c_j , which correspond to m = 5 and N = 14, are given in Tables 1 and 2.

Let us describe the error

(3.9)
$$R_m(f) = \int_a^b p(x) f(x) \, \mathrm{d}x - \sum_{j=1}^m c_j f(x_j) \, .$$

We assume to this end that the integrals (3.3) have been evaluated exactly. There are two types of estimates available [2]. In the first estimate, the 2*m*th derivative of the function f is used:

(3.10)
$$R_m^{(1)}(f) \leq Q \sup_{[a,b]} |f^{(2m)}(z)|,$$

where

$$Q = \frac{1}{(2m)!} \int_{a}^{b} p(x) \prod_{j=1}^{m} (x - x_j)^2 \, \mathrm{d}x \, .$$

In the second case the estimate is computed from the deviation between the function f(x) and its best polynomial approximation P_{2m-1} :

(3.11)
$$R_m^{(2)}(f) \leq E_{2m-1} V,$$

where

	x	С	
 1	0.1000241710 D 00	0.2516457030 D 00	_
2	0.4898873684 D 00	0.2510457059 D 00	
2	0.1065565579 D 01	0.4551871739 D 00	
4	0.1675354898 D 01	0.2370522368 D 00	
5	0.2166405047 D 01	0.4961609179 D-01	
6	0.2667972440 D 01	-0.5472173319 D-01	
7	0.3221972761 D 01	-0.2148069076 D 00	
8	0.3938251717 D 01	-0.2994195059 D 00	
9	0.4664326139 D 01	-0.1891792165 D 00	
10	0.5240787341 D 01	0.4332660401 D-01	
11	0.5789406870 D 01	0·3852548265 D-01	
12	0.6352098903 D 01	0.1562310182 D 00	
13	0.7073682880 D 01	0·2248834731 D 00	
14	0·7800726299 D 01	0·1457364120 D 00	
15	0.8375724761 D 01	0·3394592847 D-01	
16	0·8924971373 D 01	-0.3140629102 D-01	
17	0·9490388866 D 01	-0.1287239534 D 00	
18	0·1021351880 D 02	-0.1874406802 D 00	
19	0·1094043055 D 02	-0.1226933652 D 00	
20	0·1151433989 D 02	-0·2878499977 D-01	
21	0·1206369161 D 02	0·2717424411 D-01	
22	0·1263042384 D 02	0·1119712833 D 00	
23	0·1335426765 D 02	0·1640213122 D 00	
24	0·1408100449 D 02	0·1079423878 D 00	
25	0·1465422149 D 02	0·2542567487 D-01	
26	0·1520360978 D 02	-0·2429144448 D-01	
27	0·1577111291 D 02	-0.1004108830 D 00	
28	0·1649536379 D 02	-0.1476237354 D 00	
29	0·1722195602 D 02	-0-9747815354 D-01	
30	0·1779470556 D 02	-0·2301963215 D-01	
31	0·1834405936 D 02	0·2216178199 D-01	
32	0·1891207771 D 02	0·9181709331 D-01	
33	0·1963660124 D 02	0·1353261201 D 00	
34	0·2036309197 D 02	0·8956413651 D-01	
35	0·2093551574 D 02	0·2118772964 D-01	
36	0·2148496405 D 02	0·2051741592 D-01	
37	0·2205332144 D 02	-0.8511214345 D-01	
38	0·2277800449 D 02	-0·1256576199 D 00	
39	0·2350438472 D 02	-0.8330210145 D-01	
40	0·2407653930 D 02	-0·1973167732 D-01	
41	0·2462594249 D 02	0·1918536653 D-01	
42	0·2519447185 D 02	0·7968514728 D-01	

Table 1. Abscissae and coefficients of the formula for the evaluation of the integral (3.4) with n = 0. The first seventy values (which correspond to m = 5 and N = 14) are given in the semi-logarithmic form.

Table 1. Continued

	X	С
43	0-2591939514 D 02	0·1178059565 D 00
44	0·2664570898 D 02	0.7819730826 D-01
45	0·2721767393 D 02	0·1854111653 D-01
46	0·2776707773 D 02	-0·1808412531 D-01
47	0·2833591358 D 02	
48	0·2906084137 D 02	-0·1112621274 D 00
49	0·2978709833 D 02	-0.7392767339 D-01
50	0·3035890777 D 02	-0·1754225252 D-01
51	0·3090832875 D 02	0·1715414712 D-01
52	0·3147732448 D 02	0·7136170068 D-01
53	0·3220232941 D 02	0·1056991711 D 00
54	0·3292853396 D 02	0·7028766021 D-01
55	0·3350021411 D 02	0·1668905311 D-01
56	0·3404965164 D 02	-0.1635468110 D-01
57	0·3461877572 D 02	-0.6807163438 D-01
58	0·3534384026 D 02	-0·1008939763 D 00
59	0·3606999857 D 02	-0.6713649025 D-01
60	0·3664156897 D 02	-0·1594921782 D-01
61	0·3719097744 D 02	0·1565558752 D-01
62	0·3776021569 D 02	0.6519732351 D-01
63	0·3848533877 D 02	0.9669119122 D-01
64	0·3921146556 D 02	0.6437610372 D-01
65	0·3978294844 D 02	0·1530033117 D-01
66	0·4033235916 D 02	-0·1503943229 D-01
67	0·4090169082 D 02	-0.6265925745 D-01
68	0·4162686150 D 02	-0·9297279096 D-01
69	0·4235296050 D 02	-0.6192980497 D-01
70	0·4292437008 D 02	-0.1472426309 D-01

$$E_{2m-1} = \inf_{P_{2m-1}} \sup_{[a,b]} |f(x) - P_{2m-1}(x)|,$$
$$V = \int_{a}^{b} p(x) \, \mathrm{d}x + \sum_{j=1}^{m} c_j.$$

In both (3.10) and (3.11), there is an integral term independent of the integrated function f(x). The other term is determined by the function f and so we have no a priori estimate for it. In some cases something can be said about the class of functions applied in a particular field. For instance, in geophysics the majority of functions used contain an exponential term of type $\exp(-ax)$, Re a > 0. If a is not very small, it is possible to choose the number N less than 14. The roundoff error may be neglected [15].

Let us demonstrate the values of Q and V in some intervals l_i . For $p(x) = J_0(x)$:

		X	С
	1	0·3322609510 D 00	0-8787217078 D-01
	2	0·1021857833 D 01	0·3640915275 D 00
	3	0·1900917154 D 01	0.5305699045 D 00
	4	0·2785765007 D 01	0·3420420516 D 00
	5	0·3489107291 D 01	0.7818363460 D-01
	6	0-4103727573 D 01	-0-4610226904 D-01
	7	0·4673615905 D 01	-0·1849194256 D 00
	8	0·5406406934 D 01	-0·2634048159 D 00
	9	0·6146168375 D 01	-0·1692637849 D 00
	10	0·6732048574 D 01	0·3918459618 D-01
	11	0·7287922221 D 01	0·3489395037 D-01
	12	0·7856171356 D 01	0·1424113522 D 00
	13	0-8583698981 D 01	0·2064367229 D 00
	14	0.9315687059 D 01	0·1345949468 D 00
	15	0.9894011238 D 01	0·3148368521 D-01
	16	0·1044622709 D 02	0·2927230776 D-01
	17	0·1101447847 D 02	-0·1203424656 D 00
	18	0·1174067536 D 02	-0·1758418744 D 00
	19	0·1247014724 D 02	
	20	0·1304576360 D 02	0·2714871417 D-01
	21	0·1359674612 D 02	0·2572576336 D-01
	22	0·1416520116 D 02	0·1061955627 D 00
	23	0·1489092163 D 02	0·1558812069 D 00
	24	0·1561922922 D 02	0·1027790999 D 00
	25	0·1619348970 D 02	0·2424376928 D-01
	26	0.1674393155 D 02	-0·2322589481 D-01
	27	0·1731259059 D 02	-0.9612112847 D-01
	28	0·1803810542 D 02	-0.1415087701 D 00
	29	0·1876575782 D 02	-0.9355825902 D-01
	30	0·1933920946 D 02	-0·2211441103 D-01
	31	0·1988933563 D 02	0·2133928251 D-01
	32	0·2045817358 D 02	0.8847032270 D-01
	33	0·2118359518 D 02	0·1305147108 D 00
	34	0·2191083819 D 02	0·8645695333 D-01
	35	0·2248375798 D 02	0·2046664789 D-01
4.5	36	0·2303368713 D 02	-0.1984950059 D-01
	37	0·2360267824 D 02	-0.8240215846 D-01
	38	0·2432805893 D 02	-0.1217490963 D 00
	39	0·2505502625 D 02	
•	40	0·2562756985 D 02	-0·1914144317 D-01
t e	41	0·2617743721 D 02	0·1863757753 D-01
	42	0·2674654468 D 02	0·7743778373 D-01

Table 2. Abscissae and coefficients of the formula for the evaluation of the integral (3.4) with n = 1. The first seventy values (which correspond to m = 5 and N = 14) are given in the semilogarithmic form.

Table 2. Continued

	x	с
43	0·2747189554 D 02	0·1145443092 D 00
44	0·2819865173 D 02	0.7607176258 D-01
45	0·2877090770 D 02	0·1804428105 D-01
46	0·2932064125 D 02	-0-1761967074 D-01
47	0·2988986758 D 02	-0.7327439047 D-01
48	0·3061522492 D 02	0-1084895770 D 00
49	0·3134184281 D 02	-0.7211554846 D-01
50	0·3191389276 D 02	-0.1711768262 D-01
51	0·3246356857 D 02	0·1675438180 D-01
52	0·3303288427 D 02	0.6971920903 D-01
53	0-3375824097 D 02	0·1033037701 D 00
54	0·3448474260 D 02	0.6871859138 D-01
55	0·3505661775 D 02	0·1632093084 D-01
56	0·3560627593 D 02	-0·1600595055 D-01
57	0·3617566660 D 02	0.6663716463 D-01
58	0·3690102717 D 02	-0.9879797342 D-01
59	0·3762743428 D 02	-0.6576074063 D-01
60	0·3819916889 D 02	-0.1562584665 D-01
61	0·3874878889 D 02	0·1534933212 D-01
62	0·3931824907 D 02	0.6393122662 D-01
63	0·4004361750 D 02	0-9483563821 D-01
64	0·4076994970 D 02	0.6315584665 D-01
65	0·4134156954 D 02	0·1501296695 D-01
66	0·4189118096 D 02	-0·1476814704 D-01
67	0·4246069739 D 02	-0.6153066701 D-01
68	0·4318607043 D 02	-0.9131482106 D-01
69	0·4391233834 D 02	-0.6083737477 D-01
70	0·4448385840 D 02	-0·1446687094 D-01

$$\begin{split} Q &= 0.11173 \times 10^{-7}, \quad V = 0.80145 \quad \text{in} \quad l_2 = (2.4048, \quad 5.5201), \\ Q &= 0.88087 \times 10^{-8}, \quad V = 0.59932 \quad \text{in} \quad l_3 = (5.5201, \quad 8.6537), \\ Q &= 0.74228 \times 10^{-8}, \quad V = 0.49905 \quad \text{in} \quad l_4 = (8.6537, \quad 11.792). \end{split}$$

Further, for $p(x) = J_1(x)$:

$Q = 0.12135 \times 10^{-7},$	V = 0.70287	in	$l_2 = (3.8317, 7.0156),$
$Q = 0.87211 \times 10^{-8},$	V = 0.54982	in	$l_3 = (7.0156, 10.173),$
$Q = 0.72404 \times 10^{-8},$	V = 0.46806	in	$l_4 = (10.173, 13.324).$

For testing the suggested quadrature the functions have been used for which the exact values of integrals are known. For example, we have

(3.12)
$$\int_0^\infty J_0(x) \frac{x \, dx}{\sqrt{x^2 + 1} \exp \sqrt{x^2 + 1}} = 0.1719096 ,$$
$$\int_0^\infty J_1(x) \, x \, e^{-x} \, dx = 0.3535535 .$$

The results obtained by our Gaussian procedure are 0.1719312 and 0.3535531, respectively.

One of the properties of the procedure described, which is a consequence of using the Gauss quadrature (and not the Lobatto one), is that all the five abscissae lie strongly inside the interval l_i . So it is possible to use the procedure for a function f(x) with a singularity at the point x = 0. Naturally, in this case one cannot expect as exact results as in (3.12). However, for the integral

(3.13)
$$\int_0^\infty \frac{1}{x} J_1(x) \, dx = 1 \, ,$$

the approximate result was 0.95021, so the error is not more than 5%.

It may be noted that if the function f(x) has singular points then it is advisable to separate (by expansion into a power series) the terms including singularity as well as the terms slowing down the decrease of f(x) at infinity. As a rule, these terms may be integrated analytically (see, for example, (3.13)). But these problems are too far from the subject of our paper.

4. THE COMPUTATIONAL COMPARISON OF THE EFFICIENCY

The procedure described in Section 2, which consists in the evaluation of (2.2) where (2.10) is employed, gives simultaneously the values of $I_n^*(r_j)$, $j = 0, ..., N_2/2$, where the r_j 's are given by (2.9). Therefore, the computation of such a set of values of integrals served us for the comparison of the efficiency of the procedures of Sections 2 and 3.

Both the procedures have been tested on a set of simple model integrals

(4.1)
$$I_n(r_j) = \int_0^\infty \exp(-zx) J_n(r_j x) dx$$

where

$$r_j = 2\pi j / (Nh), \quad j = 0, ..., N/2,$$

with some fixed $N = 2^{\nu}$ and h. The other parameters used were n = 0 and 1, and z = 0.125, 0.5, 1, and 2. Typical values were N = 64 and h = 0.2.

The fast Fourier transform approach thus gives all the values (4.1) simultaneously if N_2 is properly chosen. The Gaussian formula was applied (N/2 + 1) times to obtain the same set of results.

In order to obtain roughly the same accuracy as with the Gaussian formula, we took $h_1 \approx 0.1$ and $N_1 \approx 150$. Further, we were forced to take $h_2 \approx 0.03$ and $N_2 \approx 2^3 N$ in the fast Fourier transform. We thus obtained simultaneously much more results than required (as far as the parameter r_j is concerned) but for a very high extra cost.

The comparison in single precision shows that the Gaussian quadrature formula is 10-20 times faster (depending on the N_1 and N_2 chosen) than the fast Fourier transform approach. It means that the work invested into the evaluation of the abscissae and coefficients of the special Gaussian formula pays.

This is the conclusion concerning the evaluation of the integral (1.1). We wish to recall that the fast Fourier transform approach is a very efficient tool when the simpler integral (1.2) is evaluated.

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Souhrn

O NUMERICKÉM VÝPOČTU INTEGRÁLŮ OBSAHUJÍCÍCH BESSELOVY FUNKCE

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Článek je věnován efektivnímu výpočtu integrálu (1.1), kde J_n je Besselova funkce nezáporného celého indexu *n*, pro zadanou posloupnost reálných parametrů $r = r_0, ..., r_J$. Jde o integrál, jehož hodnota je důležitá v řadě aplikací, např. při výpočtu hodnot elektromagnetického pole v geofyzice.

V práci jsou popsány a porovnány dva postupy, První spočívá v přímém zobecnění postupu pro výpočet integrálu (1.2) s váhovou funkcí exp (irx), který je založen na rychlé Fourierově transformaci. Druhý postup využívá konstrukce speciální kvadraturní formule Gaussova typu s váhovou funkcí J_n . Uzly a koeficienty formule jsou uvedeny v tabulkách 1 a 2.

Výsledky srovnání ukazují, že použití formule Gaussova typu je podstatně účinnější.

Резюме

О ВЫЧИСЛЕНИИ ИНТЕГРАЛОВ, СОДЕРЖАЩИХ ФУНКЦИИ БЕССЕЛЯ

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Статья посвящена эффективному вычислению интеграла $\int_0^{\infty} f(x) J_n(rx) dx$, где J_n — функция Бесселя неотрицательного целого индекса *n*, для заданной последовательности значений действительного параметра *r*.

Приводятся и сравниваются две процедуры. Одна из них заключается в прямом обобщении процедуры для вычисления родственного интеграла с весом $\exp(irx)$, которая пользуется быстрым преобразованием Фурье. Второй подход основан на построении частной квадратурной формулы типа Гаусса с весом J_n .

Результаты сравнения показывают, что применение формулы типа Гаусса гораздо более эффективно.

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