Generation of Spherical Bessel Functions in Digital Computers*

FERNANDO J. CORBATÓ

Massachusetts Institute of Technology, Cambridge, Massachusetts

AND

JACK L. URETSKY

University of California, Berkeley, California

Abstract. A method of computation for spherical Bessel functions of real and imaginary argument is given which is especially suitable for high speed digital computers. The accuracy and convergence are examined and criterion formulas are given. A procedure based on the Wronskian is used to simplify the final normalization.

1. *Introduction*

It is often the case when one attempts to solve a problem on a high speed digital computer that one finds it necessary to furnish the machine with a great many values of some well-known analytic function. There are essentially two ways to do this. One technique is to initially read a table of function values into the computer where it is kept in internal storage during the computation. Alternatively, the values of the table may be initially generated or the function values may be generated as needed within the computer.

Extensive use has been made of a function generator in connection with the solutions of the spherical Bessel equation. It turns out that in the case of these functions it is possible to formulate a method of generation which is particularly well adapted for machine use. The method is based upon the use of recurrence relations which are quite simple in form, thereby being easily coded, and yet give high numerical accuracy throughout the range of order and argument met in most applications. Of course, the use of recurrence relations implies that the method would be most efficiently utilized in those calculations where one requires the value of the function for many different orders at each specified value of the argument.

Thus the purpose of this paper is to show how the recurrence relations may be used in a straightforward manner for generating in a digital computer the various types of spherical Bessel functions. In particular, the problem of starting the recurrence relations is discussed from the viewpoint that a computer program must be able to achieve a prescribed accuracy entirely from pre-established criteria.

It will be realized that there are other functions whose behavior is such that they can be treated in a similar manner. In particular, the ratio method described

* Presented at the meeting of the Association, June 11–13, 1958. This work was sponsored in part by the Office of Naval Research under contract N5ori60 when both authors were in the Physics Department, M.I.T.

in this paper has been used for the computation of Legendre functions of integral order and argument greater than unity [1]. Similarly the cylindrical Bessel functions may be treated by the ratio method [2, 3]. Thus beyond indicating in detail the application of the ratio method to spherical Bessel functions, the principal result of the present paper lies in the specification of the starting criterion of the recurrence relations.

2. *Behavior of the Functions*

The definitions and elementary properties of the spherical Bessel functions of real argument are well-known [4]. We define the functions of imaginary argument as

$$\begin{aligned} i_n(x) &= (-i)^n j_n(ix), \\ k_n(x) &= -i^n h_n(ix). \end{aligned} \tag{1}$$

These definitions are chosen so that the functions i_n and k_n are always real and positive for positive arguments. Hereafter in this paper x will always be used to denote a real positive quantity and n an integer greater than or equal to zero.

If f_n is one of the spherical Bessel functions j_n, n_n, or h_n, it obeys the recursion relation

$$\left(\frac{2n+1}{x}\right) f_n(x) = f_{n-1}(x) + f_{n+1}(x) \tag{2}$$

and the differential equation

$$\left[\frac{d^2}{dx^2} + 1 - \frac{n(n+1)}{x^2}\right][x f_n(x)] = 0. \tag{3}$$

It follows from the differential equation that the transition line $x^2 = n(n+1)$ separates two regions of the $x - n$ plane in which the functions j_n and h_n have essentially different behavior. Below the transition line, where $n(n+1)$ is less than x^2, the functions $j_n(x)$ and $h_n(x)$ behave as oscillating functions of both order and argument. Above the transition line, however, the behavior becomes monotonic and it is possible to prove the following inequalities:

$$\begin{aligned} \frac{j_{n+1}(x)}{j_n(x)} &< \frac{x}{n+3}, \qquad \text{for} \quad n(n+1) > x^2 \\ \frac{h_{n+1}(x)}{h_n(x)} &> \frac{n-1}{x}, \qquad \text{for} \quad n(n+1) > x^2, \quad n > 1 \end{aligned} \tag{4}$$

The proof of these inequalities follows from the behavior of the functions for small x and the integral relations [4]:

$$\begin{aligned} \int x^{n+1} f_n(x)\, dx &= x^{n+2} f_{n+1}(x) \\ \int x^{1-n} f_n(x)\, dx &= -x^{1-n} f_{n-1}(x) \end{aligned} \tag{5}$$

The hyperbolic functions $i_n(x)$ and $k_n(x)$ are monotonic functions of n as well as of x so that

$$\begin{aligned} i_n(x) &> i_{n+1}(x) > 0, \\ k_{n+1}(x) &> k_n(x) > 0. \end{aligned} \tag{6}$$

3. *Computational Procedure*

We now consider the problem of computing a set of one of the functions $j_n(x)$, $h_n(x)$, $i_n(x)$, $k_n(x)$ for several contiguous orders and a given value of the argument. We continue to require that the argument be positive; this introduces no loss in generality since the first three functions are either even or odd in their argument while the fourth satisfies

$$k_n(-x) = -2i_n(x) - (-1)^n k_n(x). \tag{7}$$

It is immediately seen that for the two functions h_n and k_n, which increase (or at worst, oscillate) with increasing order, use of the recursion relation (2) is trivial. The initial values at orders zero and one are readily calculated in terms of sines and cosines or exponentials. Upward recursion is an accurate process in this case.

A similar method cannot be used for the remaining two functions since upward recursion (except in the region of the $x - n$ plane where the j_n oscillate or where the i_n have asymptotic form for large x) would bring about a rapid loss of accuracy resulting from cancellations. In both cases downward recursion is called for, and the computational problem reduces to that of determining the initial conditions for the corresponding recursion relation. It should be noted that recursion in the oscillatory region of j_n is essentially a fixed-point process and not particularly sensitive to the direction of recursion. Similarly either direction of recursion of the i_n in the asymptotic region, where x is large compared to n, is accurate in the sense that the upward cancellations do not seriously affect the accuracy.

In order to describe the downward recursion process by the ratio method [1], we will discuss the computation of the functions $j_n(x)$ for a definite value of x and all orders from zero to some N such that $N(N + 1) > x^2$. It will be shown that rather than accurately evaluate $j_N(x)$ and $j_{N-1}(x)$ to start the process, a technique of very approximately starting the recursion at a higher order will give a set of numbers which are accurately proportional to the j_n (i.e., the ratios are accurate) over the desired range of n from 0 to N.

We first choose some integer ν, which is larger than N, and two arbitrary positive numbers which will be denoted by $\bar{j}_\nu(x)$, $\bar{j}_{\nu+1}(x)$. It follows from the nonvanishing of the Wronskian that there exist an α and β such that

$$\begin{aligned} \bar{j}_{\nu+1}(x) &= \alpha[j_{\nu+1}(x) + \beta n_{\nu+1}(x)], \\ \bar{j}_\nu(x) &= \alpha[j_\nu(x) + \beta n_\nu(x)]. \end{aligned} \tag{8}$$

By using the barred quantities as initial conditions for the recursion relation

(2), we can find a new number

$$\bar{j}_N(x) = \alpha j_N(x)\,[1 - \epsilon]. \tag{9}$$

Making the special choice of $\bar{j}_{\nu+1}$ equal to zero, it follows from the inequalities (4) that

$$\epsilon < x^{2(\nu-N+1)}\,\frac{(N+2)!(N-2)!}{(\nu+3)!(\nu-1)!}, \tag{10}$$

so that by choosing ν sufficiently larger than N we can make the barred and unbarred quantities as nearly proportional as we please. In figure 1 we give a plot of $\nu - N$ arising from expression (10) when it is taken as an equality and ϵ is set equal to 2^{-30}. In practice, of course, the choice of ν is made inside the computer by evaluating the right side of expression (10) with successively increasing trial values of ν until the expression is less than a given maximum value of ϵ.

Using the numbers $\bar{j}_N(x)$, $\bar{j}_{N-1}(x)$ obtained by the method just discussed, we can now resort to the recursion relation (2) to find a set of numbers $\bar{j}_n(x)$ each element of which is accurately proportional to $j_n(x)$ in the interval $0 \leqq n \leqq N$.

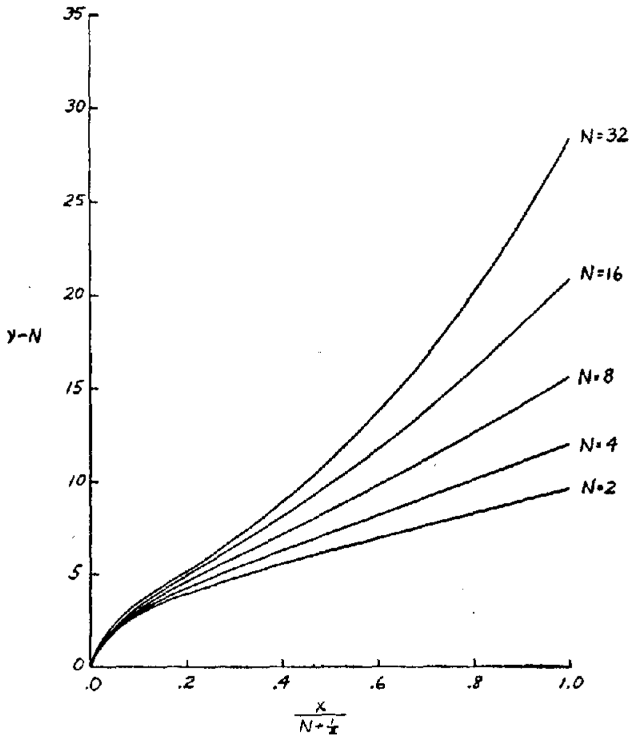

FIG. 1. Plot of $\nu - N$ versus $x/(N + \frac{1}{2})$ arising from expression (10) when it is taken as an equality and ϵ is set equal to 2^{-30}.

The constant of proportionality is readily obtained from the relation

$$\alpha = (\bar{j}_0 - x\bar{j}_1)\cos x + x\bar{j}_0 \sin x. \tag{11}$$

The corresponding relation for the i_n is

$$\alpha = e^{-|x|}[(1 + |x|)\,\bar{\imath}_0 + x\bar{\imath}_1]. \tag{12}$$

Relations (11) and (12) have the virtue of being numerically accurate for all finite x. This allows the use of a single formula for each normalization which is a major advantage in computer coding.

The expressions for α are obtained by use of the Wronskian and explicit forms for order zero and one. Thus if $\bar{j}_n = \alpha j_n$, the Wronskian of the functions of real argument may be written as

$$\alpha^{-1}[\bar{j}_0(x)h_1(x) - \bar{j}_1(x)h_0(x)] = -ix^{-2},$$

where

$$h_0(x) = -i\frac{e^{ix}}{x}, \qquad h_1(x) = -\left(\frac{i + x}{x^2}\right)e^{ix}. \tag{13}$$

Upon substitution expression (11) follows directly.

There are other normalization techniques which may be useful under special conditions. One might extend the recursion relation (2) to define a function

$$j_{-1}(x) = -h_0(x) = \frac{\cos x}{x} \tag{14}$$

and normalize by using the explicit form of $j_0(x)$ or $j_{-1}(x)$, whichever is necessary since either of these functions may vanish for certain values of x.

Alternatively, one might utilize the addition theorem for spherical Bessel functions which states that

$$\sum_{n=0}^{\infty}(2n + 1)\,[j_n(x)]^2 = 1. \tag{15}$$

Saffren has found this method useful in computations where the required number of orders is sufficient so that the indicated summation is convergent [5].

In a similar manner the normalization constant, α, for the i_n functions is determined from the Wronskian written as

$$\alpha^{-1}\,[\bar{\imath}_0(x)k_1(x) + \bar{\imath}_1(x)k_0(x)] = x^{-2}. \tag{16}$$

Substitution of the explicit forms

$$k_0(x) = \frac{e^{-x}}{x}, \qquad k_1(x) = \frac{e^{-x}}{x^2}(1 + x) \tag{17}$$

leads to equation (12), where the absolute value signs maintain a numerically accurate form for negative arguments.

As with the j_n, there are alternative normalization procedures. Use may be made of the explicit form

$$i_0(x) = \frac{\sinh x}{x}, \tag{18}$$

but this requires special numerical treatment for the case of arguments near or equal to zero. The addition theorem normalizations based on

$$\sum_{n=0}^{\infty} (-1)^n(2n + 1)[i_n(x)]^2 = 1 \tag{19}$$

or

$$\sum_{n=0}^{\infty} (2n + 1)\, i_n(x) = e^x \tag{20}$$

are not entirely satisfactory since in the first the alternating signs will cause loss of numerical accuracy, and in the second the slow convergence for large x may present difficulties.

In the process of coding the above recursive technique for the M.I.T. Whirlwind Computer it was found necessary to introduce certain modifications. The reason for these changes was that the function j_n grows so rapidly with decreasing n (above the transition line) that there was danger of generating numbers too large to be stored in the computer during the recursion process. In order to avoid this difficulty we worked with the ratios $\bar{r}_n = \bar{j}_{n+1}/\bar{j}_n$ using the same recursion relation as for the ratios $r_n = j_{n+1}/j_n$:

$$\bar{r}_{n-1} = \frac{x}{2n + 1 - x\bar{r}_n}, \tag{21}$$

but with the initial condition $\bar{r}_\nu$ equal to zero where ν is defined as before. Recursion is continued downward until a ratio is reached, say $\bar{r}_\lambda$, which exceeds unity, indicating that the transition line has been passed. At this point we make the convenient choice $\bar{j}_{\lambda+1} = \bar{r}_\lambda$, $\bar{j}_\lambda = 1$, and continue downward using the recursion relation (2). This switch avoids the possibility of computing excessively large ratios in the vicinity of the zeros of the function which occur below the transition line. Obviously no such switching from the ratio recursion relation need be made with the i_n functions which never oscillate.

It should be noted that the efficiency of the above computational process depends on the ability of the generator program in the computer to determine a value of ν which is safely high enough for the accuracy desired. For this purpose it is also possible to make an error analysis in terms of the ratios instead of dealing directly with the functions as we have done. The analysis leads to an alternate criterion for determining the initial order ν.

We begin by examining the propagation of error in the continued fraction equation (21). Suppose, then that we have $\bar{r}_n$ which differs from the ratio r_n by a fractional error, ϵ_n, and we ask for the resultant error, ϵ_{n-1}, in r_{n-1}. Using (21)

$$(1 - \epsilon_{n-1})r_{n-1} = \frac{x}{2n + 1 - (1 - \epsilon_n)xr_n} = \frac{r_{n-1}}{1 + \epsilon_n\, r_n\, r_{n-1}} \tag{22}$$

in the monotonic region where the ratios are less than unity and assuming the errors are small, it follows that

$$\epsilon_{n-1} \cong \epsilon_n r_{n-1} r_n , \qquad n \geqq N. \tag{23}$$

The latter expression may be used to derive the error ϵ_N obtained when $\bar{r}_\nu$ is taken as zero:

$$\epsilon_N \cong \prod_{k=N+1}^{\nu} r_{k-1} r_k < r_N^{2(\nu-N)} = \bar{r}_N^{2(\nu-N)}, \tag{24}$$

where it is assumed that $\bar{r}_N$ is accurate enough to replace r_N. It should be emphasized that although for typical N the values of $r_{\nu-1}$ and r_ν are small compared to unity, expression (22) and hence (23) will not be rigorously true since $\epsilon_\nu = 1$. However, for typical N the convergence is rapid so that the error is usually small in the expression (24) for ϵ_N. Since the subsequent argument will only utilize the inequality of expression (24), the resultant approximate upper bound for ν, which will be developed, will usually be a true upper bound. Thus to establish the validity of the final result for the upper bound of ν it is necessary to check the worst-convergent case, in particular, to check the accuracy of $r_N(\sqrt{N(N+1)})$ for the maximum N to be used.

The expression (24) may next be manipulated into a more convenient form. We define $\tilde{r}_n$ as the solution of

$$\tilde{r}_n = \frac{x}{2n + 1 - x\tilde{r}_n}. \tag{25}$$

which vanishes for vanishing x. It can be shown by induction from $\bar{r}_\nu = 0$ that $\tilde{r}_n > \bar{r}_{n-1} > \bar{r}_n$. Hence by replacing $\bar{r}_N$ in the inequality (24) by the explicit solution for $\tilde{r}_N$ from equation (25), one arrives at

$$\nu - N < \frac{-\ln \epsilon_N}{2 \sinh^{-1} [(u^{-2} - 1)^{\frac{1}{2}}]}, \qquad u = \frac{2x}{2N+1}. \tag{26}$$

By graphical means it is easily shown that for all positive t

$$\frac{\ln 2}{2 \sinh^{-1} t} < A + Bt^{-1} \tag{27}$$

where $A = .10$, $B = .35$.

Utilizing this expression and the inequality,

$$\frac{1 - u^2}{1 - (1/2)u^2} \leqq 1 - u^2, \quad (u^2 \leqq 1) \tag{28}$$

yields

$$\nu - N < -\log_2 \epsilon_N \left[A + \frac{Bu(2 - u^2)}{2(1 - u^2)} \right]. \tag{29}$$

If the last inequality is taken as an equality with ν replaced by ν_1, then ν_1 is an upper bound for ν. The expression for ν_1 may be further improved by considering

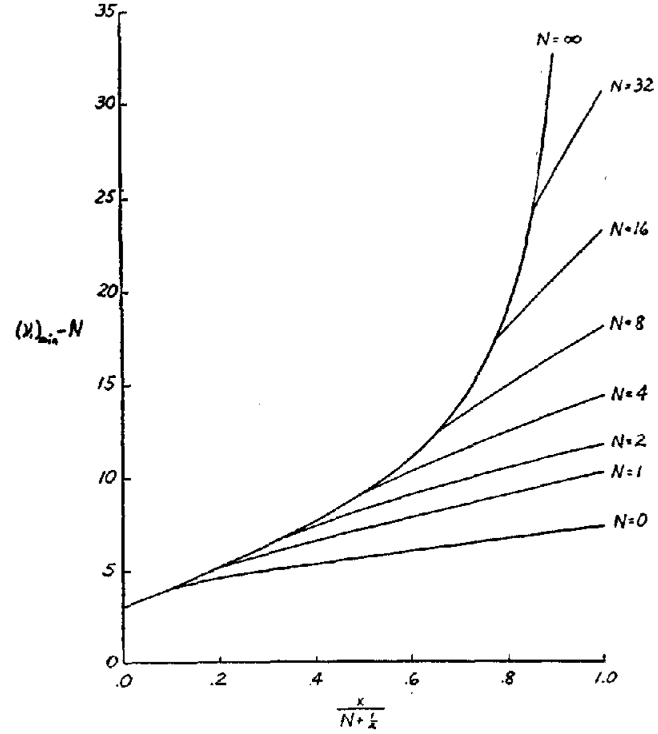

FIG. 2. Plot of $(\nu_1)_{min} - N$ versus $x/(N + \frac{1}{2})$ from equation (31) when ϵ_N is set equal to 2^{-30}.

ν_1 as a function of x and N. There then exists the possibility that a larger value of N, which we designate N', will yield a lower value of ν_1, namely $(\nu_1)_{min}$. Rather than differentiate with respect to N the equation for ν_1 to determine N', it is algebraically simpler to consider a further weakening of inequality (29) which yields the following simplified equality when ν is replaced by ν_2:

$$\nu_2 = N - \log_2 \epsilon_N \left[A + \frac{Bu}{1 - u} \right]. \tag{30}$$

Minimization of ν_2 with respect to N (subject to the constraint that $N' \geqq N$) then yields a value for N' which roughly (and adequately) minimizes the expression (29) for ν_1. When this is done one obtains the final expression

$$(\nu_1)_{min} = N' - \log_2 \epsilon_N \left[A + \frac{Bu'(2 - u'^2)}{2(1 - u'^2)} \right], \tag{31}$$

where $u' = 2x/2N' + 1$ and N' is either N or $x - \frac{1}{2} + [(-\log_2 \epsilon_N)Bx]^{\frac{1}{2}}$, the choice being determined by whichever value gives the lower value of $(\nu_1)_{min}$, subject only to the constraint that $N' \geqq N$.

The quantity $(\nu_1)_{min}$ is plotted in figure 2 for the special case where $\epsilon_N = 2^{-30}$.

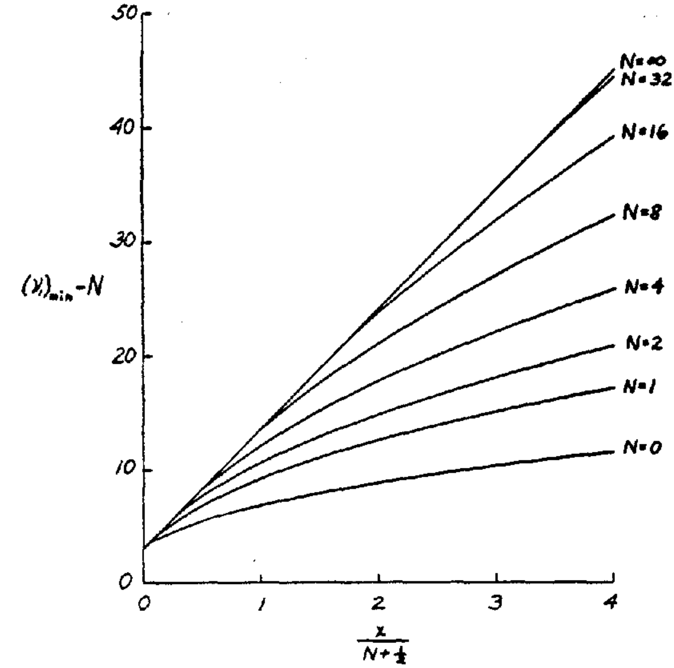

FIG. 3. Plot of $(\nu_1)_{min} - N$ versus $x/N + \frac{1}{2})$ from equation (33) when ϵ_N is set equal to 2^{-30}.

This value was deliberately chosen for use in connection with the M.I.T. Whirlwind Computer which can conveniently store floating point numbers with a 30 binary digit mantissa. Clearly, the quantity $(\nu_1)_{min}$ is not difficult to evaluate inside a computer, so that it offers an alternative procedure to the use of expression (10) described earlier.

A very similar analysis may be performed for determining the starting order ν_1 of the downward recursion process of the hyperbolic spherical Bessel functions i_n, [6]. One obtains

$$\nu - N < \frac{-\ln \epsilon_N}{2 \sinh^{-1} u} < (-\log_2 \epsilon_N)(A + Bu). \tag{32}$$

Minimization with respect to N yields the result

$$(\nu_1)_{min} = N' + (-\log_2 \epsilon_N)\ (A + Bu'), \tag{33}$$

where $u' = 2x/(2N' + 1)$ and N' is the greater of N or $-\frac{1}{2} + [(-\log_2 \epsilon_N)Bx]^{\frac{1}{2}}$. Figure 3 is a plot of $(\nu_1)_{min}$ of equation (33), $(\epsilon_N = 2^{-30})$, for the range $0 \leqq u \leqq 4$ where the i_n cannot be accurately recursed upward by means of the relation

$$\left(\frac{2n+1}{x}\right) i_n(x) = i_{n-1}(x) - i_{n+1}(x). \tag{34}$$

In conclusion it is seen that expressions (10), (31) and (33) offer useful upper-bounds for the starting order ν in the downward recursion processes. Thus these expressions offer an alternative to the other possible procedures of repeatedly recursing from trial ν values until effective convergence is achieved or of partially parametizing ν from an empirical determination of the function $\nu(x, N, \epsilon_N)$.

REFERENCES

1. As M. Abramowitz has kindly pointed out to us, the earliest known application of the ratio method of recursion with unnormalized functions rather than with the functions themselves is found in: J. C. P. MILLER, British Association for the Advancement of Science, Mathematical Tables, Vol. X, *Bessel Functions, Part II*, University Press (Cambridge) 1952, p. xvi.
2. The ratio method was used for desk calculation by C. W. JONES, *A Short Table for the Bessel Functions* $I_{n+\frac{1}{2}}(x)$, $(2/\pi)K_{n+\frac{1}{2}}(x)$, University Press, Cambridge (1952).
3. The ratio method for the generation of the cylindrical functions $J_n(x)$ and $Y_n(x)$ is described by: J. B. RANDELS AND R. F. REEVES, *Communications ACM*, *1* (May 1958).
4. P. M. MORSE AND H. FESHBACH, *Methods of Theoretical Physics*, McGraw-Hill (New York) 1953, p. 1573.
5. M. SAFFREN, Physics Department, Massachusetts Institute of Technology, Cambridge, Mass. (private communication).
6. In the case of the $i_n(x)$ a weaker expression for ν_1 is given by: F. J. CORBATÓ, *J. Chem. Phys.* *24*, 452 (1956).