JOURNAL OF COMPUTATIONAL PHYSICS 8, 162–166 (1971)

Note

On the Use of Recursion Relations in the Numerical Evaluation of Spherical Bessel Functions and Coulomb Functions*

The regular and irregular spherical Bessel functions, $j_l(\rho)$ and $n_l(\rho)$ are often needed for fixed ρ and for various orders, l. This situation arises, for example, in the scattering of electromagnetic waves or in a potential scattering problem in quantum mechanics [1]. In this case it is natural to evaluate the Bessel functions by recursion relation. The irregular function $n_l(\rho)$ can be obtained from the known values of $n_0(\rho) = -\cos(\rho)/\rho$ and $n_1(\rho) = -\cos(\rho)/\rho^2 - \sin(\rho)/\rho$ by the recursion relation $n_{l+1}(\rho) = (2l + 1)\, n_l(\rho)/\rho - n_{l-1}(\rho)$ beginning with $l = 1$ and recurring in the direction of increasing order l. However, it is now well known that the regular function cannot be obtained in this manner because this "forward" recursion is unstable when l is greater than ρ [2]. It is also well known that the regular functions can be obtained by using the relation backwards. That is, if we know $j_l(\rho)$ and $j_{l+1}(\rho)$ for some l the relation

$$j_{l-1}(\rho) = (2l + 1)\, j_l(\rho)/\rho - j_{l+1}(\rho) \tag{1}$$

used toward smaller l is a stable method. The problem is to determine $j_l(\rho)$, $j_{l+1}(\rho)$ for some order l.

Consider the functions $F_l(\rho) \equiv \rho j_l(\rho)$ and $G_l(\rho) \equiv -\rho n_l(\rho)$. They satisfy the same recursion relation as $j_l(\rho)$ and $n_l(\rho)$. They also satisfy the Wronskian relation

$$F_l(\rho)\, G_{l+1}(\rho) - G_l(\rho)\, F_{l+1}(\rho) = 1 \tag{2}$$

or

$$F_l(\rho)/G_l(\rho) - F_{l+1}(\rho)/G_{l+1}(\rho) = 1/G_l(\rho)\, G_{l+1}(\rho). \tag{3}$$

Writing this down for one higher l value

$$F_{l+1}(\rho)/G_{l+1}(\rho) - F_{l+2}(\rho)/G_{l+2}(\rho) = 1/G_{l+1}(\rho)\, G_{l+2}(\rho) \tag{4}$$

and adding the two equations, one obtains

$$F_l(\rho)/G_l(\rho) - F_{l+2}(\rho)/G_{l+2}(\rho) = \sum_{i=l}^{l+1} 1/G_i(\rho)\, G_{i+1}(\rho). \tag{5}$$

Work supported in part by the National Science Foundation.

Continuing this procedure one derives the relation

$$F_l(\rho)/G_l(\rho) = \sum_{i=l}^{\infty} 1/G_i(\rho)\, G_{i+1}(\rho), \tag{6}$$

since

$$F_{l+k}(\rho)/G_{l+k}(\rho) \to 0 \qquad \text{as} \quad k \to \infty \qquad \text{for fixed } \rho.$$

Suppose one needs $F_l(\rho)$, $G_l(\rho)$ for $l = 0, 1,..., L$. First form $G_l(\rho)$ for $l = 0,..., L$ using the recursion relation. Next keep recuring the $G_l(\rho)$ functions and form the sum that appears in the Wronskian formula. This sum is rapidly convergent as soon as l is greater than ρ. Calling the sum in Eq. (6), S one has

$$F_L(\rho) = G_L(\rho) \cdot S \tag{7}$$

and

$$F_{L-1}(\rho) = G_{L-1}(\rho) \cdot S + 1/G_L(\rho). \tag{8}$$

Now the backward recursion relation can be used to determine all $F_l(\rho)$ for $l = L - 2, L - 3,..., 0$.

The following table shows the formation of the sum for the case $\rho = 10$ and $L = 14$. Here the $G_l(\rho)$ are obtained from $G_0(10) = -0.83907153$ and $G_1(10) = -0.62793826$.

i	$1/G_i(10)G_{i+1}(10)$	S
14	$1.5302377.10^{-3}$	$1.5302377.10^{-3}$
15	$2.3327075.10^{-4}$	1.7635084
16	$2.9614871.10^{-5}$	1.7931233
17	$3.2020033.10^{-6}$	1.7963253
18	$2.9963224.10^{-7}$	1.7966249
19	$2.4569613.10^{-8}$	1.7966495
20	$1.7832239.10^{-9}$	1.7966513
21	$1.1551602.10^{-10}$	1.7966514

Then $F_{14}(10) = 2.9410783.10^{-2}$ and $F_{13}(10) = 7.4655845.10^{-2}$ are found since $G_{14}(10) = 1.6369777.10^{1}$ and $G_{13}(10) = 7.5516370$ are known from forward recursion. The correct value of $F_0(10) = \sin(10) = -.54402111$ is then obtained by backward recursion. Notice that the terms in the sum are decreasing more than one order of magnitude from one value of i to the next.

If one needs $F_l(\rho)$ for $l = 0, 1, 2,..., L$, where $L < \rho$ they can be formed by forward recursion. Nevertheless it is interesting to ask if the present method would have any difficulty in that case. It would then be possible for a $G_i(\rho)$ to be zero in the sum of Eq. (6) and the equation would be incorrect. However, this can easily be remedied by noting that the offending factor appears in two terms

$$1/G_{i-1}(\rho)\, G_i(\rho) + 1/G_i(\rho)\, G_{i+1}(\rho)$$

and that this expression can be rewritten as $(2i+1)/\rho G_{i-1}(\rho)\, G_{i+1}(\rho)$ by using the recursion relation. Thus such a factor can be easily removed.

The most commonly used method of obtaining $F_L(\rho)$, $F_{L-1}(\rho)$ to begin the backward recursion is the Miller technique [1]. In this procedure one guesses $F_{N+1}(\rho) = 0$ for some $N \gg L$. Then the downward recursion relation is used to find all $F_l(\rho)$. These must then be normalized by the known value of $F_0(\rho)$. But how does one choose N such that the relative error of $F_{L-1}(\rho)$ and $F_L(\rho)$ is negligible? N clearly depends on both L and ρ. The empirical procedure most often used here is to guess an N, calculate all F_l, guess a larger N and recalculate the F_l and see if they agree for $l = 0, 1, 2,..., L$; See Refs. [3, 4]. If not, repeat with still a larger N until the $F_l(\rho)$ have converged. Both the iterative nature of this procedure and the normalization can be avoided if the currently proposed procedure is used.

Mechel [5] has provided a significant improvement over Miller's technique in obtaining $F_L(\rho)$ and $F_{L-1}(\rho)$. His approach is to recognize that the recursion relation, Eq. (1), can be written as

$$\rho F_{L-1}(\rho)/F_L(\rho) = (2L+1) - \rho^2/\rho F_L(\rho)/F_{L+1}(\rho) \tag{9}$$

and that for $L > \rho$ this can be evaluated by the continued fraction

$$\rho F_{L-1}(\rho)/F_L(\rho) = (2L+1) - \frac{\rho^2}{2L+3\,-}\;\frac{\rho^2}{2L+5\,-}\;\frac{\rho^2}{2L+7}\cdots. \tag{10}$$

Knowing the ratio of $F_{L-1}(\rho)$ to $F_L(\rho)$, the set of F_l generated by downward recursion are only unknown by a common constant factor. This factor is obtained by the known value of $F_0(\rho)$, as in the Miller technique. In evaluating the continued fraction one does not know in advance how many terms to include, to obtain a given accuracy in the $F_l(\rho)$. Thus, the sum will have to be done at least twice to check for accuracy. This recalculation of the sum and the required normalization are avoided in the method proposed in this paper.

Mechel's method and the present method using Eqs. (6)–(8) were compared for the case $\rho = 10$, $l = 0, 1, 2,..., 14$. Both methods were programmed in FORTRAN 4 for the Indiana University CDC 6600 computer. The code using the proposed method was 145 words long and took 1.02 μsec. to compute $F_l(\rho)$ and $G_l(\rho)$. The program using Mechel's method was 137 words long and took 0.90 μsec. to compute $F_l(\rho)$ alone. A simple program to calculate G_l alone was 63 words long and took

0.33 μsec. It is seen that Mechel's method has a slight advantage if only the regular functions are needed and that the proposed method has an advantage if both the regular and irregular functions are needed. In his paper Mechel suggests that $F_L(\rho)$ be computed by the approximate relation $F_L(\rho) \approx 1/G_{L+1}(\rho)$, which is the first term of the sum in Eq. (6). The value of this procedure is to get the normalization about correct to avoid overflow. If this procedure is followed, then the set of $G_l(\rho)$ have to computed and his method would lose its advantage over Eq. (6). However, the relation he suggests is only a relation between the first terms of the power series expansions for $F_L(\rho)$ and $G_{L+1}(\rho)$, thus one can write $F_L(\rho) \approx \rho^{L+1}/(2L+1)!!$ and avoid the calculation of $G_{L+1}(\rho)$.

The discussion thus far has considered only the spherical Bessel functions. The Coulomb wavefunctions satisfy a similar Wronskian relation

$$F_l(\eta, \rho)/G_l(\eta, \rho) = \sum_{i=l}^{\infty} A_{i+1}/G_i G_{i+1} \tag{11}$$

with

$$A_i = i/[i^2 + \eta^2]^{1/2}.$$

Here the normalization is

$$F_l(\eta, \rho) \to \sin \theta_l\,, \qquad G_l(\eta, \rho) \to \cos \theta_l \qquad \text{as} \quad \rho \to \infty$$

with

$$\theta_l = \rho - \eta Ln(2\rho) - l\pi/2 + \sigma_l \qquad \text{and} \quad \sigma_l = \arg \Gamma(l + 1 + i\eta).$$

The computation of $G_0(\eta, \rho)$ and $G_1(\eta, \rho)$ is much more difficult in this case but once that is done the use of the Wronskian relation to determine $F_l(\eta, \rho)$ for some large l is the same as for Bessel functions. The Coulomb wavefunction programs described by Smith [3] and Tamura [4] still use the Miller approach. They could be improved by using the present method.

It is also noted that the method of Mechel can be applied to Coulomb functions yielding

$$H_L(\rho) = (2L + 1)(\eta\rho + L(L + 1))/(L(L + 1)) - (1 + \eta^2/(L + 1)^2)\, \rho^2/H_{L+1}(\rho), \tag{12}$$

where $H_L(\rho) = (1 + \eta^2/L^2)^{1/2}\, \rho F_{L-1}(\rho)/F_L(\rho)$. The normalization is more difficult here than in the case of spherical Bessel functions.

References

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Received: December 7, 1970

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