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ON THE COMPUTATION OF RICCATI-BESSEL FUNCTIONS

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Summary. The paper deals with the computation of Riccati-Bessel functions. A modification of Miller method is presented together with estimates of relative errors.

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Scattering of electromagnetic radiation from a sphere, the so-called Mie scattering, requires the computation of Riccati-Bessel functions [2, 3, 5].

Riccati-Bessel functions are functions ψ_n and χ_n defined recursively by the formulas

$$\psi_0(x) = \sin x\,, \tag{1.a}$$

$$\chi_0(x) = \cos x\,, \tag{1.b}$$

$$\psi_1(x) = \frac{\sin x}{x} - \cos x\,, \tag{2.a}$$

$$\chi_1(x) = \frac{\cos x}{x} + \sin x\,, \tag{2.b}$$

$$\psi_{n+1}(x) = \frac{2n+1}{x}\,\psi_n(x) - \psi_{n-1}(x)\,, \tag{3.a}$$

$$\chi_{n+1}(x) = \frac{2n+1}{x}\,\chi_n(x) - \chi_{n-1}(x)\,. \tag{3.b}$$

It is known that the computation of ψ_n by formulas (1.a)–(3.a) is highly unstable. On the other hand, the computation of χ_n by formulas (1.b)–(3.b) is stable. These facts are explained below.

Since the functions ψ_n can not be computed by upward recurrence for large n, they are usually computed by downward recurrence. This, the so-called Miller method, is described in [1], pp. 206–7 and 270–1 for functions J_n and j_n. (The connection between j_n and ψ_n is given by formula (5.a) below.)

The idea of the Miller method is as follows. For sufficiently large N we put $\tilde{\psi}_{N+1} = 0$, $\tilde{\psi}_N = 1$, and $\tilde{\psi}_n$ are computed by downward recurrence, i.e.,

$$\tilde{\psi}_{n-1} = \frac{2n+1}{x}\tilde{\psi}_n - \tilde{\psi}_{n+1}\,. \tag{4}$$

The values $\psi_n(x)$ may be obtained from $\tilde{\psi}_n$ after multiplication by a constant C, the value of which may be found as $\psi_0/\tilde{\psi}_0$ (or $\psi_1/\tilde{\psi}_1$ when ψ_0 is near to 0).

The present paper gives a modification of the Miller method. This modification is useful in the case when the values χ_n are also required (they are computed by upward recurrence). For sufficiently large N we put

$$\tilde{\psi}_N = 0\,, \quad \tilde{\psi}_{N-1} = 1/\chi_N$$

and $\tilde{\psi}_n$ are computed by (4). No multiplication is necessary, because there is an effective estimate of $|\tilde{\psi}_n/\psi_n - 1|$ in terms of χ_n. This estimate gives a possibility to determine N in the case when the required accuracy of the computation is given.

1. ELEMENTARY PROPERTIES OF RICCATI-BESSEL FUNCTIONS

Riccati-Bessel functions ψ_n and χ_n are connected with Bessel functions $J_{n+1/2}$ and $Y_{n+1/2}$ and spherical Bessel functions j_n and y_n by the formulas

$$\psi_n(x) = x\,j_n(x) = \sqrt{\left(\frac{\pi x}{2}\right)}\,J_{n+1/2}(x)\,, \tag{5.a}$$

$$\chi_n(x) = -x\,y_n(x) = -\sqrt{\left(\frac{\pi x}{2}\right)}\,Y_{n+1/2}(x)\,. \tag{5.b}$$

The functions ψ_n and χ_n may be expressed as the series

$$\psi_n(x) = \sum_{k=0}^{\infty} \frac{(-1)^k\,x^{2k+n+1}}{(2k)!!\,(2k+2n+1)!!}\,, \tag{6.a}$$

$$\chi_n(x) = \sum_{k=0}^{\infty} \frac{(-1)^{n+k}\,x^{2k-n}}{(2k)!!\,(2k-2n-1)!!}\,. \tag{6.b}$$

Relations (6.a) and (6.b) follow directly from the recurrence formulas (1)–(3). For analogous expressions for j_n and y_n see [1], p. 256.

Note that

$$(2k)!! = 2\cdot 4\cdot\ldots\cdot 2k\,,$$
$$(2k+1)!! = 1\cdot 3\cdot\ldots\cdot(2k+1)\,,$$
$$(-1)!! = 1\,,$$
$$(-2k-1)!! = \frac{(-1)^k}{(2k-1)!!}\,.$$

Relations (6.a) and (6.b) are not good for the evaluation when n is large, but they imply the asymptotical behaviour of ψ_n and χ_n

$$\psi_n(x) \sim \frac{x^{n+1}}{(2n+1)!!}, \tag{7.a}$$

$$\chi_n(x) \sim \frac{(2n-1)!!}{x^n} \tag{7.b}$$

when x is fixed and $n \to \infty$ or n is fixed and $x \to 0$. (The symbol $\sim$ means that the limit of the quotient of both sides is 1.) It means that the asymptotical behaviour of ψ_n and χ_n is determined by the initial term of series (6).

Relations (7) may be deduced also from the behaviour of J_ν and Y_ν given in [1], p. 187 and [4], p. 548.

We suppose that x is a fixed positive number and we write ψ_n and χ_n instead of $\psi_n(x)$ and $\chi_n(x)$ if it causes no confusion.

Proposition 1. *Functions ψ_n and χ_n satisfy the relations*

$$\begin{vmatrix} \psi_n & \chi_n \\ \psi_{n+1} & \chi_{n+1} \end{vmatrix} = \psi_n\chi_{n+1} - \psi_{n+1}\chi_n = 1 \quad \text{for all} \quad n. \tag{8}$$

If $n + \frac{1}{2} > x$, then

(9.a) $\psi_n > 0$, (9.b) $\chi_n > 0$,

(10.a) $\psi_n > \psi_{n+1}$, (10.b) $\chi_n < \chi_{n+1}$,

$$\frac{1}{\chi_{n+1}} < \psi_n < \frac{1}{\chi_{n+1} - \chi_n}, \tag{11}$$

$$\chi_{n+1} - \chi_n > \chi_n - \chi_{n-1}. \tag{12}$$

Proof. Relation (8) follows from (1)–(3) by induction. The functions $\psi_n(x)$ and $\chi_n(x)$ have a constant sign when $x \in (0, n + \frac{1}{2})$, because the smallest positive zero of the functions J_ν and Y_ν is greater than ν [6], p. 385 and 387. Relations (7) show that the functions $\psi_n(x)$ and $\chi_n(x)$ are positive for small x. This proves relations (9.a) and (9.b).

Suppose that for some $n_0 > x - \frac{1}{2}$ we have $\psi_{n_0+1} \geqq \psi_{n_0}$. Then relation (3.a) gives $\psi_{n+1} \geqq \psi_n$ for all $n \geqq n_0$. But this is impossible, because $\lim_{n\to\infty} \psi_n(x) = 0$ by (7.a).

Now, we shall prove (10.b). The function $J_\nu^2(x) + Y_\nu^2(x)$ is an increasing function of the parameter ν when x is fixed. This follows from the integral representation of this function in [6], p. 444. It means that the sequence $\{\psi_n^2 + \chi_n^2\}_{n=0}^\infty$ is increasing. Using (9.a), (9.b) and (10.a) we obtain (10.b).

Relation (8) gives $\psi_n\chi_{n+1} = 1 + \psi_{n+1}\chi_n$. If $n + \frac{1}{2} > x$, then we have $\psi_n\chi_{n+1} > 1$ and $\psi_n\chi_{n+1} < 1 + \psi_n\chi_n$ by (9) and (10). The last inequalities imply (11).

If $n + \frac{1}{2} > x$, then $\chi_{n+1} = (2n + 1)\chi_n/x - \chi_{n-1} > 2\chi_n - \chi_{n-1}$, which implies (12).

2. COMPUTATION OF RICCATI-BESSEL FUNCTIONS

Now, we shall explain why the computation of $\psi_n(\chi_n)$ by upward recurrence is unstable (stable). This fact is well known and it is presented only for the sake of completeness.

Suppose that the values ψ_n are computed by formulas (1.a)–(3.a). Owing to the rounding error the computed values $\tilde{\psi}_n$ and the actual ones ψ_n are generally different. Let $\tilde{\psi}_n = (1 + \alpha_n)\psi_n$, i.e., the relative error of the computation ψ_n is α_n. To see the behaviour of relative errors better we will assume that the equality $\tilde{\psi}_{n+1} = (2n + 1) \,.\, \tilde{\psi}_n/x - \tilde{\psi}_{n-1}$ holds exactly for $n \geqq N + 1$ where N is fixed. Then three sequences $\{\psi_n\}_{n=N}^{\infty}$, $\{\chi_n\}_{n=N}^{\infty}$ and $\{\tilde{\psi}_n\}_{n=N}^{\infty}$ are solutions of the recurrence equation $u_{n+1} = (2n + 1)u_n/x - u_{n-1}$.

Since $\{\psi_n\}_{n=N}^{\infty}$ and $\{\chi_n\}_{n=N}^{\infty}$ are linearly independent by (8), $\{\tilde{\psi}_n\}_{n=N}^{\infty}$ must be a linear combination of $\{\psi_n\}_{n=N}^{\infty}$ and $\{\chi_n\}_{n=N}^{\infty}$, i.e., $\tilde{\psi}_n = A\psi_n + B\chi_n$ for all $n \geqq N$, where A and B are constants. From the initial conditions

$$\begin{aligned} \tilde{\psi}_N &= (1 + \alpha_N)\psi_N\,, \\ \tilde{\psi}_{N+1} &= (1 + \alpha_{N+1})\psi_{N+1} \end{aligned}$$

we obtain a system of linear equations

$$\begin{aligned} \psi_N A + \chi_N B &= (1 + \alpha_N)\psi_N\,, \\ \psi_{N+1}A + \chi_{N+1}B &= (1 + \alpha_{N+1})\psi_{N+1}\,. \end{aligned}$$

The Cramer rule and relation (8) give

$$\begin{aligned} A &= 1 + (\alpha_N\psi_N\chi_{N+1} - \alpha_{N+1}\psi_{N+1}\chi_N) \quad \text{and} \\ B &= (\alpha_{N+1} - \alpha_N)\psi_N\psi_{N+1}\,. \end{aligned}$$

It means that for all $n \geqq N$

$$\tilde{\psi}_n = \psi_n + (\alpha_N\psi_N\chi_{N+1} - \alpha_{N+1}\psi_{N+1}\chi_N)\psi_n + (\alpha_{N+1} - \alpha_N)\psi_N\psi_{N+1}\chi_n$$

and

$$\alpha_n = \frac{\tilde{\psi}_n}{\psi_n} - 1 = (\alpha_N\psi_N\chi_{N+1} - \alpha_{N+1}\psi_{N+1}\chi_N) + (\alpha_{N+1} - \alpha_N)\psi_N\psi_{N+1}\frac{\chi_n}{\psi_n}\,.$$

Using (7) we obtain $\lim_{n\to\infty}|\alpha_n| = \infty$ whenever $(\alpha_{N+1} - \alpha_N)\psi_N\psi_{N+1} \neq 0$. It means that in the general case the relative error of ψ_n tends to infinity even in the case when the computation is exact for $n \geqq N + 1$. This shows that the computation of ψ_n by upward recurrence is unstable.

Now, suppose that

$$\tilde{\chi}_n = (1 + \beta_n)\,\chi_n \qquad \text{for all} \quad n \geqq 0 \quad \text{and}$$

$$\tilde{\chi}_{n+1} = \frac{2n+1}{x}\,\tilde{\chi}_n - \tilde{\chi}_{n-1} \quad \text{for all} \quad n \geqq N + 1 \, .$$

Then we obtain (by the same method as before)

$$\tilde{\chi}_n = \chi_n + (\beta_{N+1}\psi_N\chi_{N+1} - \beta_N\psi_{N+1}\chi_N)\,\chi_n + (\beta_N - \beta_{N+1})\,\chi_N\chi_{N+1}\psi_n \, ,$$

$$\beta_n = \frac{\tilde{\chi}_n}{\chi_n} - 1 = (\beta_{N+1}\psi_N\chi_{N+1} - \beta_N\psi_{N+1}\chi_N) + (\beta_N - \beta_{N+1})\,\chi_N\chi_{N+1}\frac{\psi_n}{\chi_n}$$

for all $n \geqq N$.

Since $\lim_{n\to\infty} \psi_n/\chi_n = 0$ by (7), the sequence $\{\beta_n\}_{n=N}^{\infty}$ is bounded. Moreover, there are constants K and L such that $|\beta_n| \leqq K|\beta_N| + L|\beta_{N+1}|$ for all $n \geqq \max\,(x - \frac{1}{2}, N)$. We see that the computation of χ_n by upward recurrence is stable.

Assume that the values χ_n are computed for $n = 0, \ldots, N + 1$ by upward recurrence, where N is sufficiently large. Put

$$\tilde{\psi}_N = 0 \, , \tag{13}$$

$$\tilde{\psi}_{N-1} = 1/\chi_N \tag{14}$$

and compute $\tilde{\psi}_n$ by downward recurrence (4). Then $\tilde{\psi}_n = A\psi_n + B\chi_n$ (if the rounding error is neglected). Relations (13), (14) and (8) imply $A = 1$ and $B = -\psi_N/\chi_N$. Hence

$$\tilde{\psi}_n = \psi_n - (\psi_N/\chi_N)\,\chi_n \, . \tag{15}$$

Take $\tilde{\psi}_n$ as an approximation of ψ_n. Denote by γ_n the relative error of this approximation. Then

$$\gamma_n = \frac{\tilde{\psi}_n}{\psi_n} - 1 = -\frac{\psi_N\chi_n}{\chi_N\psi_n} \, . \tag{16}$$

Using (11) we obtain the following theorem.

Theorem 1. *The relative error γ_n satisfies the inequality*

$$|\gamma_n| \leqq \frac{\chi_n\chi_{n+1}}{\chi_N(\chi_{N+1} - \chi_N)} \tag{17}$$

whenever $N \geqq n > x - \frac{1}{2}$.

Now, suppose that for some $n_0 > x - \frac{1}{2}$ it is necessary to compute ψ_{n_0} so that $|\gamma_{n_0}| \leqq \gamma$ where $\gamma > 0$ is prescribed. We find the minimal index N such that

$$(18) \qquad \frac{\chi_{n_0}\chi_{n_0+1}}{\chi_N(\chi_{N+1} - \chi_N)} \leqq \gamma .$$

(The existence of N follows from (9.b), (10.b), (12) and (7.b).) If we start downward recurrence from this index N, then for all n between n_0 and $x - \frac{1}{2}$ we shall have $|\gamma_n| \leqq \gamma$. It follows from (10.b), (17) and (18).

We shall give another estimate of the relative error which may be used for all n. Relation (15) implies

$$\psi_n = \tilde{\psi}_n + \frac{\psi_N}{\chi_N}\chi_n$$

and

$$\frac{\psi_n}{\tilde{\psi}_n} - 1 = \frac{\psi_N}{\chi_N}\frac{\chi_n}{\tilde{\psi}_n} .$$

Relation (11) gives

$$(19) \qquad \left|\frac{\psi_n}{\tilde{\psi}_n} - 1\right| \leqq \frac{1}{\chi_N(\chi_{N+1} - \chi_N)}\left|\frac{\chi_n}{\tilde{\psi}_n}\right| .$$

Note that $|(\psi_n/\tilde{\psi}_n) - 1|$ and $|(\tilde{\psi}_n/\psi_n) - 1|$ are nearly the same if one of them is small.

Relations (16), (11), (1) and (2) yield the following estimates for γ_0 and γ_1:

$$(20) \qquad |\gamma_0| \leqq \frac{|\text{cotg}\, x|}{\chi_N(\chi_{N+1} - \chi_N)} ,$$

$$(21) \qquad |\gamma_1| \leqq \frac{1}{\chi_N(\chi_{N+1} - \chi_N)}\frac{|1 + x\,\text{tg}\, x|}{|\text{tg}\, x - x|} .$$

If $\frac{1}{2} > x > 0$, we may use inequality (17) for the estimate of γ_0 and γ_1. If $x > \frac{1}{2}$ we may use (20) and (21), Since $\chi_N(\chi_{N+1} - \chi_N)$ is large, $|\gamma_0|$ may be large if and only if $|\text{tg}\, x|$ is small. (It means that γ_0 may be large if and only if $\psi_0 = \sin x$ is small.) But in this case $|\gamma_1|$ is small. This shows why no multiplication is necessary.

For the absolute error of ψ_0 we have the estimate

$$(22) \qquad |\psi_0 - \tilde{\psi}_0| \leqq \frac{|\cos x|}{\chi_N(\chi_{N+1} - \chi_N)} \leqq \frac{1}{\chi_N(\chi_{N+1} - \chi_N)} .$$

Remark. The estimates (17), (19), (20), (21) and (22) are based on neglecting the rounding error. They consider only the error which is caused by approximations (13) and (14).

The method presented here was tested on EC 1033 by the authors. No rounding error was observed. The equalities

$$\psi_n\chi_{n+1} - \psi_{n+1}\chi_n = 1 \quad \text{and} \quad \psi_0 = \sin x$$

were satisfied up to 12 significant digits.

Partial results are summarized in the table. For given x, n_0 denotes the minimal n for which $\chi_n > 10^{12}$. N is chosen so that $|\gamma_{n_0}| < 10^{-13}$.

Table

x	n_0	N
0.001	4	6
0.01	6	8
0.1	8	11
1	14	18
10	33	41
100	147	162
1000	1100	1131

References

[1] *M. Abramowitz, I. A. Stegun:* Handbook of mathematical functions with formulas, graphs and mathematical tables. Washington, National Bureau of Standards, 1964 (Russian translation, Moskva, Nauka, 1979).

[2] *C. F. Bohren, D. R. Huffman:* Absorption and Scattering of Light by Small Particles. J. Wiley, New York 1983 (Russian translation, Moskva, Mir, 1986).

[3] *M. Kerker:* The Scattering of Light and Other Electromagnetic Radiation. Academic Press, New York 1969.

[4] *V. I. Smirnov:* Kurs vyssej matematiki. Tom III. Časť 2. Moskva, Nauka, 1974.

[5] *H. C. van de Hulst:* Light Scattering by Small Particles. J. Wiley, New York 1957 (Russian translation, Moskva, Inostrannaja literatura, 1961).

[6] *G. N. Watson:* A Treatise on the Theory of Bessel Functions. University Press, Cambridge 1945.

Súhrn

VÝPOČET RICCATIHO-BESSELOVÝCH FUNKCIÍ

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Článok sa zaoberá výpočtom Riccatiho-Besselových funkcií spätnou rekurziou. Sú v ňom odvodené niektoré nerovnosti pre Riccatiho-Besselove funkcie a odhady chýb pri numerických výpočtoch.

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