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A SIMPLIFICATION OF LENTZ'S ALGORITHM

AUGUST 1982

By

W. J. Lentz

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A SIMPLIFICATION OF LENTZ'S ALGORITHM

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Page 7, sixth line from bottom of page, change ". . . and the denominator [-1,1]" to ". . . and the denominator [1,-1]"

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20. ABSTRACT (*Continue on reverse side if necessary and identify by block number*) The Lentz algorithm is a method of computing the continued fraction representation of functions. It was originally developed to calculate spherical Bessel functions in Mie scattering calculations. A simplification of the algorithm improvement is presented for the case in which a given term is exactly zero. A FORTRAN IV program is presented which calculates three test cases correctly when the numerator or denominator terms are exactly zero.		

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CONTENTS

INTRODUCTION

The ratios of spherical Bessel functions of complex argument are needed for Mie calculations of scattering and absorption. Lentz has developed a new continued fraction technique[1] for evaluating these ratios, with an improvement to eliminate errors when certain terms approach or become zero. The authors of a recent note,[2] however, had difficulty in applying the algorithm improvement when either the numerator or denominator was exactly zero. This case is special, and a simplification is possible. The purpose of this paper is to present an algorithm for this special case, together with some clarifying remarks concerning its development.

BACKGROUND

The Lentz algorithm is simply a way of calculating continued fractions; the algorithm begins at the beginning of the continued fraction rather than at some indeterminate final coefficient. An improvement formula allows one to bypass any step in which a given numerator or denominator might be zero (to the accuracy of the computer). In addition, roundoff errors may be reduced by using the algorithm improvement. When applied to the continued fraction representation of ratios of Bessel functions, the method is easy to use and free of most of the weaknesses of the other algorithms used to generate ratios of Bessel functions.[2]

Let us review the method of computing a continued fraction by defining the simple continued fraction. The simple continued fraction is defined for arbitrary a_n not equal to zero as

$$F = a_1 + \cfrac{1.0}{a_2 + \cfrac{1.0}{a_3 + \cfrac{1.0}{a_4 + \dots}}} , \qquad (1)$$

which may be written as

$$F = a_1 + \frac{1}{a_2 +} \frac{1}{a_3 +} \frac{1}{a_4} + \dots , \qquad (2)$$

and the n'th partial convergent of the continued fraction is

---

[1] Lentz, W. J., "Generating Bessel Functions in Mie Scattering Calculations Using Continued Fractions," Applied Optics, 15:668, 1976.

[2] Jaaskelainen, T., and J. Ruuskanen, "Note on Lentz's Algorithm," Applied Optics, 20:19, 1981.

$$F_n = a_1 + \frac{1}{a_2} + \frac{1}{a_3} + \frac{1}{a_4} + \frac{1}{\ldots} + \frac{1}{a_n} \, . \qquad (3)$$

The Lentz algorithm is simply a way of computing the F_n without starting at some indeterminate last a_n. A further simplification of notation is needed:

$$F_n = [a_1, a_2, \ldots, a_n] \, . \qquad (4)$$

Then the Lentz algorithm becomes

$$F_n = \frac{[a_1]\,[a_2, a_1]\,[a_3, a_2, a_1] \ldots [a_n, a_{n-1}, \ldots, a_1]}{[a_2]\,[a_3, a_2] \ldots \qquad [a_n, a_{n-1}, \ldots, a_2]} \, . \qquad (5)$$

Although the formula looks complicated, the successive numerators and denominators are generated by taking the reciprocal of the previous numerator or denominator and adding it to the next a_m.

When a given numerator is equal to its corresponding denominator (to the number of digits accuracy that is desired), the continued fraction is said to have converged.

Original Algorithm Improvement

The original algorithm paper included an improvement technique to avoid inaccuracy when any term in the numerator or denominator approached or became zero. The problem step is bypassed without loss of accuracy even if the term is exactly zero. Consider the following case in which $1/\alpha$ is equal to but of opposite sign to a_m. When a_m is added to $1/\alpha$, every digit that is the same in the two terms will cancel and cause a loss of accuracy in the final number if no steps are taken to bypass the problem. For example,

Let $[a_{m-1}, \ldots, a_1] = \alpha$

If $[a_m, \ldots, a_1] = \beta = a_m + 1/\alpha \to 0$

and $[a_{m+1}, \ldots, a_1] = \gamma = a_{m+1} + 1/\beta \to \infty$

so $[a_{m+2}, \ldots, a_1] = Z = a_{m+2} + 1/\gamma$

Then $\xi = \beta\gamma = \beta \, \dfrac{a_{m+1}\,\beta + 1}{\beta} = a_{m+1}\,\beta + 1 \qquad (6)$

where ξ is not necessarily 1.0.

The product of the two terms $\beta\gamma = \xi$ can be correctly calculated by equation (6). This avoids the problem of multiplying zero times infinity in equation (5).

ξ is the product of the next two terms. z, the next numerator or denominator, is then

$$z = \frac{a_{m+2}\ \gamma + 1}{\gamma} = \frac{a_{m+2}\ (a_{m+1}\ \beta + 1) + \beta}{a_{m+1}\ \beta + 1}$$
$$= \frac{a_{m+2}\ \xi + \beta}{\xi} = a_{m+2} + \beta/\xi\ . \tag{7}$$

The algorithm improvement may be applied to the denominator by replacing a_1 by a_2 in the above equations. The algorithm improvement may be applied independently to either the numerator or denominator or to both.

Numerical Examples

Consider the following three cases, which illustrate the implementation of the normal Lentz algorithm and the Lentz algorithm with improvement.

Case A: $F_{na} = \sqrt{2} = [1,2,2,2,2,\ldots]$

$$= \frac{1 *\ 3 *\ 2.333 * 2.428571429 *\ 2.411764706 *\ 2.414634146}{2 * 2.5 * 2.4 * 2.4166666666 * 2.413793103} \ldots$$

Case B: $F_{nb} = [1,1,-1,1,2] = 0.5$

Case C: $F_{nc} = [1,-1,1,-1,2] = 0.5$

In case B the denominator [-1,1] is exactly zero, regardless of the computer word length. In case C both the numerator [-1,1] and the denominator [-1,1] are zero, causing both the numerator product and the denominator product to be zero. For case B one has:

$$F_{nb} = \frac{[1]\ [1,1]\ [-1,1,1]\ [1,-1,1,1]\ [2,1,-1,1,1]}{[1]\ [-1,1]\ [1,-1,1]\ [2,1,-1,1]}$$

Applying the algorithm improvement one has

$$F_{nb} = \frac{[1]\ [1,1]\ [-1,1,1]\ [1,-1,1,1]\ [2,1,-1,1,1]}{1\ (1*0+1)\ (2+0/1)}$$

where (1*0+1) corresponds to equation (6) and (2+0/1) corresponds to equation (7). The continued fraction is then calculated with ease:

$$F_{nb} = \frac{1 * 2 * -0.5 * -1 * 1}{1 * 1 * 2} = 0.5$$

In like manner, the improvement may be applied to more complicated cases, such as case C, where corrections in both the numerator and denominator are required:

$$F_{nc} = \frac{[1]\ [-1,1]\ [1,-1,1]\ [-1,1,-1,1]\ [2,-1,1,-1,1]}{[-1]\ [1,-1]\ [-1,1,-1]\ [2,-1,1,-1]} .$$

In this case we have

$$F_{nc} = \frac{1 * (1*0+1)\ (-1+0/1)\ (2+1/-1)}{(-1)\ (-1*0+1)\ (2+0/1)} = 0.5 .$$

Notice that the term ξ cannot be zero unless $a_{m+3} = 0$, which is not allowed by definition. If any a_m were zero in the derivation of a representation of a function, the fraction could easily be transformed to the form of equation (2) by formula (5) of section 3.10.1 of Abramowitz.[3]

Up to this point we have not considered the Bessel functions for which the Lentz algorithm was derived. Like Florida orange juice for breakfast, the algorithm is not just for Bessel functions anymore. Rather, it is a general way of computing the continued fraction representation of any function. A good source of continued fraction representations of functions is found in Abramowitz together with the general properties of the functions.

DISCUSSION OF THE SIMPLIFICATION

Simplified Error Removal

In some cases it may not be desirable to include an error correction when β approaches zero but is not identically zero. When either the numerator or denominator is zero to the accuracy of the computer, a significant simplification in programming is possible. This simplification reduces the

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[3] Abramowitz, M. and I. A. Stegun, ed., Handbook of Mathematical Functions, US Department of Commerce, National Bureau of Standards, Washington, DC, 20402.

complexity of the algorithm and will often speed up its execution with little loss of accuracy.

Consider equations (6) and (7) when β is exactly zero:

$$[a_m, \ldots, a_1] = \beta = 0$$

$$[a_{m+1}, \ldots, a_1] = \gamma = a_{m+1} + 1.0/\beta$$

$$[a_{m+2}, \ldots, a_1] = z = a_{m+2} + \beta/\xi = a_{m+2} \ . \qquad (8)$$

And the product of the two terms $\beta\gamma$ is
$z = \beta\gamma = a_{m+1}\beta + 1 = 1$.

To include the simplified algorithm improvement, simply do not take the reciprocal of the previous numerator and denominator before adding the next a_{m+2}. The running product is multiplied by one, so that it does not change if the error bypass is implemented. This simplification was first published in the Hewlett Packard 67 User's Library under Spherical Bessel functions.[*] The User's Library program is no longer available, but the algorithm in appendix A details the methods used in that program.

SUMMARY

The original algorithm improvement in the computation of continued fractions may be applied to both the numerator and denominator of equation (5). A simplified version of the improvement may be implemented in the case of a numerator or denominator being exactly zero. A FORTRAN IV program implementing these ideas is listed for ease in use.

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[*] Lentz, W. J., Hewlett Packard 67/97 User's Library, No 00642.

APPENDIX A
FORTRAN IV PROGRAM SIMPLE.FR

Algorithm Example

The implementation of the simplified form of the algorithm improvement given in equations (6) and (7) can be elusive. The best method to avoid pitfalls is to check the algorithm against well-defined cases such as Case B and Case C. The FORTRAN IV program Simple.FR, listed in appendix A, correctly calculates cases A, B, and C. The program was implemented on a Data General Nova 3 minicomputer using FORTRAN V revision 6.11. The nonstandard accept and type statements allow input and output in arbitrary format and may be replaced by read and write statements in standard FORTRAN IV. The variables have the following functions:

AN = the input terms of the continued fraction from equation (4)

NUM = the current partial numerator in equation (5)

DEN = the current partial denominator in equation (5)

PDT = the n'th convergent of the continued fraction formed [illegible] the n numerators and n-1 denominators in equation (5)

NFLAG = switch to avoid taking the reciprocal of zero in the [illegible]rator

DFLAG = switch to avoid taking the reciprocal of zero in the denominator

ICOUNT = counter to keep track of the current AN

SIMPLE.FR

```
C       PROGRAM SIMPLE IS DESIGNED TO HAVE SEPARATE LOOPS FOR NUM AND DEN
C       A SIMPLIFIED TEST IS MADE FOR NUMERATOR AND DENOMINATOR EQUAL TO ZERO
C       PROGRAM PASSES THE TEST OF THE FOLLOWING SERIES
C       [1,1,-1,1,2]=0.5 AT THE LAST CONVERGENCE
C       [1,-1,1,-1,2]=0.5 AT THE LAST CONVERGENCE
C       THE FIRST TESTS THE DENOMINATOR BYPASS, AND THE SECOND THE NUMERATOR
C       BYPASS.
C*****************************************************************************
        REAL PDT,NUM,DEN,AN
C**************PROGRAM START**************************************************
1       TYPE "ICOUNT=0, INPUT AN"
        ACCEPT AN
        PDT=AN
        NUM=1./AN
        DEN=0.0
        ICOUNT=0
        NFLAG=0
        DFLAG=0
C*********MAIN LOOP POINT AFTER INITIALIZATION*******************************
10      IF(NUM.EQ.DEN.AND.NFLAG.NE.1.AND.DFLAG.NE.1)TYPE "FRACTION HAS CONVERGED"
        ICOUNT=ICOUNT+1
        TYPE "PDT=",PDT,ICOUNT
        TYPE "INPUT AN"
        ACCEPT AN
        IF(AN.EQ.0) GOTO 1
C       STOP IF AN IS ZERO WHICH IS NOT ALLOWED IN THE ALGORITHM
C*****TEST FOR PREVIOUS NUMERATOR OR DENOMINATOR ZERO. IF SO SKIP STEP********
        IF(NFLAG.NE.1) NUM=NUM+AN
        IF(DFLAG.NE.1) DEN=DEN+AN
        NFLAG=NFLAG+1
        DFLAG=DFLAG+1
C***************FOLLOWING IS NORMAL NUMERATOR LOOP UNLESS ZERO*****************
        IF(NUM.EQ.0) GOTO 11
        PDT=PDT*NUM
        NUM=1.0/NUM
        NFLAG=0
C*****************FOLLOWING IS DENOMINATOR LOOP********************************
11      IF(DEN.EQ.0) GOTO 10
        PDT=PDT/DEN
        DEN=1.0/DEN
        DFLAG=0
        GOTO 10
        END
```

```
IDENTIFIER                          REFERENCES

AN         9    12   13   14   24   25   28   29
DEN        9    15   26   29   38   39   40
DFLAG      18   20   29   31   41
ICOUNT     16   21   22
NFLAG      17   20   28   30   36
NUM        9    14   20   26   33   34   35
PDT        9    13   22   34   39

1          11   25
10         20   39   42
11         33   38
SIMPLE
ICOUNT=0, INPUT AN
1.
PDT=     0.100000E  1        1
INPUT AN
1.
PDT=     0.200000E  1        2
INPUT AN
-1.
PDT=    -0.100000E  1        3
INPUT AN
1.
PDT=     0.100000E  1        4
INPUT AN
2.
PDT=     0.500000E  0        5
INPUT AN
0
ICOUNT=0, INPUT AN
1.
PDT=     0.100000E  1        1
INPUT AN
-1.
PDT=    -0.100000E  1        2
INPUT AN
1.
PDT=    -0.100000E  1        3
INPUT AN
-1.
PDT=     0.100000E  1        4
INPUT AN
2.
PDT=     0.500000E  0        5
INPUT AN
0
ICOUNT=0, INPUT AN
```

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