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PROGRAMS FOR COMPUTING THE LOGARITHM OF THE GAMMA FUNCTION, AND THE DIGAMMA FUNCTION, FOR COMPLEX ARGUMENT

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PROGRAM SUMMARY

Title of program: CLOGAM AND CDIGAM

Catalogue number: ACRG

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: CDC 6600, *Installation*: CERN, Geneva

Operating system: CDC scope

Programming languages used: FORTRAN IV

High speed store required: 334 (CLOGAM), 232 (CDIGAM) words. *No. of bits in a word*: 60

Is the program overlaid? No

No. of magnetic tapes required: None

What other peripherals are used? Line Printer

No. of cards in combined program and test deck: 161

Card punching code: BCD

Keywords: General Purpose, Nuclear, Atomic, Gamma Function, Logarithm of Gamma Function, Psi Function, Digamma Function, Asymptotic Expansion, Coulomb, Phase Shift, Scattering, Schrödinger

Nature of the physical problem

The gamma function $\Gamma(z)$, its logarithm $\ln \Gamma(z)$, and its logarithmic derivative $\psi(z) = d \ln \Gamma(z)/dz$ appear in a wide range of physical applications. We mention here only the Veneziano model and its generalizations in high-energy physics, and the Coulomb phase shift for complex energies.

Method of solution

For $\mathrm{Re}\, z \geqslant 7$, the asymptotic expansions are used to compute $\ln \Gamma(z)$ and $\psi(\bar{z})$. For other regions of the z plane, suitable functional relations are used. Care is taken that $\mathrm{Im} \ln \Gamma(z)$ is computed correctly, and not merely modulo 2π.

Restrictions on the complexity on the problem

As the tests show, an accuracy of 12–14 significant digits is normally obtained.

Running time

Typical running times (in microseconds on the CDC 6600) are given in table 1.

Table 1

	$\ln \Gamma(z)$ (CLOGAM)	$\psi(z)$ (CDIGAM)
$\mathrm{Re}\, z < -6$	580	570
$-6 \leqslant \mathrm{Re}\, z < 0$	790	650
$0 \leqslant \mathrm{Re}\, z < 7$	630	390
$7 \leqslant \mathrm{Re}\, z$	330	300

LONG WRITE-UP

1. Introduction

Let $z = x + iy$ be a complex variable. The gamma function (for notation see [1])

$$\Gamma(z) = \int_0^\infty t^{z-1}\, e^{-t}\, dt \qquad (x > 0)\,, \tag{1}$$

its logarithm $\ln \Gamma(z)$, and the repeated derivations of $\ln \Gamma(z)$, namely

$$\psi^{(n)}(z) = \frac{d^{n+1}}{dz^{n+1}} \ln \Gamma(z) \qquad (n = 0, 1, 2, 3, \ldots) \tag{2}$$

play an important role in several fields of mathematics, physics, and other applications. The $\psi^{(n)}(z)$ are often called polygamma functions. In particular, for $n = 0$,

$$\psi(z) = \Gamma'(z)/\Gamma(z) \tag{3}$$

is called the digamma or psi function.

Several methods have been suggested for the computation of these functions, for real or complex values of the variable [2–18]. Algol programs for $\Gamma(x)$ with x real are given in [4, 5, 8, 10]; for $\ln \Gamma(x)$ in [9, 10]; and for $\psi^{(n)}(x)$ in [11]. Rational Chebyshev approximations for $\ln \Gamma(x)$ are given in [14]. For complex values of the variable z, FORTRAN programs for $\Gamma(z)$ have been published in [18] and [19]*. In a recent paper, Luke [13] treated the computation of $\Gamma(z)$ for complex z with the help of Padé approximations. He also announced publication of a program for $\Gamma(z)$ using this technique. Wrench [16] and Spira [17] have developed explicit numerical expressions for the coefficients in the Stirling series of $\Gamma(z)$. For the cases where only a limited accuracy is required, Lanczos [6] gave a remarkably simple formula for $\Gamma(z)$, namely

$$\Gamma(z) \approx (z+1)^{z-\frac{1}{2}}\, e^{-(z+1)}\, (2\pi)^{\frac{1}{2}} \times (0.999779 + 1.084635/z)\,, \tag{4}$$

which has a relative error not exceeding 2.4×10^{-4} everywhere in $\mathrm{Re}\, z > -1$, $z \neq 0$.

A 12-decimal table of $\ln \Gamma(z)$ for $x = 0(0.1)10$, $y = 0(0.1)10$ has been published by the National bureau of Standards [20]. This table also contains a compilation of properties of $\Gamma(z)$ and a bibliography.

An increasing number of applications require the computation of the functions mentioned above for complex arguments. For example, the Veneziano model and its generalizations in high-energy physics [21–23], which make extensive use of $\Gamma(z)$, or the computation of Coulomb wavefunctions for complex energies [19].

Although programs for $\Gamma(z)$ are available, it is often desirable to have a program for $\ln \Gamma(z)$. Occasionally, the derivative of the gamma function is also needed. It is therefore useful to present programs for computation of $\ln \Gamma(z)$ and $\psi(z) = \Gamma'(z)/\Gamma(z)$ for complex arguments z.

2. Methods of computation

2.1. *CLOGAM, the program for* $\ln \Gamma(z)$

Since $\ln \Gamma(z)$ is an elementary function of $\Gamma(z)$, one might ask why a separate routine is needed if one has a program for $\Gamma(z)$. The answer to this question is twofold: firstly, because the complex logarithm is a multivalued function, defined for $z = x + iy = |z| \exp[i(\theta + 2n\pi)]$ by

$$\ln z = \ln |z| + i(\theta + 2n\pi). \tag{5}$$

The standard FORTRAN function CLOG, however, usually computes only the principal value of $\ln z$, i.e., it assumes $n = 0$ and gives θ between $-\pi$ and π. This is not always sufficient if we wish to take the logarithm of a function. For example, we find from a table [20] that for $z = 1 + 5i$, $\mathrm{Im} \ln \Gamma(z) = 3.82 > \pi$, so that the FORTRAN combination CLOG(CGAMMA(Z)) would certainly not provide the right answer, assuming that CGAMMA computes $\Gamma(z)$. Unfortunately, the authors of [19] did not take this phenomena into account when using their routine GAMMA as part of their program for calculating the Coulomb phase shift. We note here that Luke [13] has

* This routine occasionally gives wrong results, a correction has been published in Computer Phys. Commun. 3 (1972) 276.

developed a method for finding Im $\Gamma(z)$ if z and $\Gamma(z)$ are given, which can also be applied to $\ln\Gamma(z)$.

The second reason for introducing a separate routine for $\ln\Gamma(z)$ is that this function is much less affected by overflow than $\Gamma(z)$. It can therefore be used for calculating quotients of gamma functions in cases where both numerator and denominator would cause overflow, but not the quotient itself.

In order to compute $\ln\Gamma(z)$, we use the Stirling series of $\ln\Gamma(z)$ together with suitable functional relations. Other formulae could also be used, for instance the logarithmic equivalent of the relations given by Lanczos [6], which are reproduced in [12]. In contrast to $\Gamma(z)$, where the Stirling series falls off like $1/z$, this series falls off like $1/z^2$ in the case of $\ln\Gamma(z)$. We then have the following formulae [12] in the different regions of the z plane:

$$\begin{aligned}\ln\Gamma(z) &= (z-\tfrac{1}{2})\ln z - z - \tfrac{1}{2}\ln 2\pi \\ &\quad + z\sum_{k=1}^{K}\frac{B_{2k}}{2k(2k-1)}z^{-2k} + R_K(z) \quad (x \geqslant x_0 > 0), \\ &= \ln\Gamma(z+n) - \ln\prod_{\nu=0}^{n-1}(z+\nu) \quad (0 \leqslant x < x_0), \\ &= \ln\pi - \ln\Gamma(1-z) - \ln\sin\pi z \quad (x<0).\end{aligned} \tag{6}$$

where $n = [x_0] - [x]$. The B_{2k} are the Bernoulli numbers, $[x]$ is the largest integer $\leqslant x$. Recently, Spira [17] proved a very simple upper bound of the remainder $R_K(z)$ in (6), namely

$$\begin{aligned}|R_K(z)| &\leqslant |B_{2K}/(2K-1)|/|z|^{1-2K} \\ &\leqslant |B_{2K}/(2K-1)|/|x|^{1-2K} \quad (x \geqslant 0).\end{aligned} \tag{7}$$

If we choose $K = 10$ and $x_0 = 7$, we find

$$|R_{10}(7)| < 2.5 \times 10^{-15}$$

so that theoretically these values are suitable for single precision computation on a CDC 6000 computer.

When computing the logarithm of the product in formula (6), we must be careful to find the correct imaginary part. This can be achieved by using the relation

$$\ln\prod_{\nu=0}^{n-1}(z+\nu) = \tfrac{1}{2}\ln\left|\prod_{\nu=0}^{n-1}(z+\nu)\right| + \mathrm{i}\sum_{\nu=0}^{n-1}\arctan\frac{y}{x+\nu}. \tag{8}$$

The function $f(z) = \ln\sin\pi z$ in formula (6) is computed in the following way. We set $z = x + \mathrm{i}y$ and assume $y \geqslant 0$. This is no restriction since $\ln\Gamma(\bar{z}) = \overline{\ln\Gamma(z)}$, where $\bar{z} = x - \mathrm{i}y$. We introduce a new variable $\xi = x - [x]$ so that $0 \leqslant \xi < 1$, and obtain

$$\begin{aligned}f(z) &= \tfrac{1}{2}\ln(\sin^2\pi\xi + \sinh^2\pi y) \\ &\quad + \mathrm{i}\,\{\arctan(\cot\pi\xi\tanh\pi y) - [x]\pi\},\end{aligned} \tag{9}$$

where $-\pi < \arctan\omega \leqslant \pi$. In particular, on the boundaries of the cut along the negative real axis ($y = \pm 0$), we have

$$f(x) = \ln|\sin\pi\xi| \mp [x]\pi\mathrm{i} = \ln|\sin\pi\xi| \pm |[x]|\pi\mathrm{i}. \tag{10}$$

Finally, in order to avoid possible overflow, we write $\operatorname{Re} f(z)$ in the form

$$\operatorname{Re} f(z) = \pi y + \tfrac{1}{2}\ln\left[\mathrm{e}^{-2\pi y}\sin^2\pi\xi + \tfrac{1}{4}\left(1-\mathrm{e}^{-2\pi y}\right)^2\right] \tag{11}$$

2.2. *CDIGAM, the program for $\psi(z)$**

In order to compute $\psi(z) = \mathrm{d}\ln\Gamma(z)/\mathrm{d}z$ we differentiate (6), giving

$$\begin{aligned}\psi(z) &= \ln z - \frac{1}{2z} - \sum_{k=1}^{K}\frac{B_{2k}}{2k}z^{-2k} + R_K'(z) \\ &\qquad\qquad (x \geqslant x_0 > 0), \\ &= \psi(z+n) - \sum_{\nu=0}^{n-1}(z+\nu)^{-1} \quad (0 \leqslant x < x_0), \\ &= \psi(-z) + 1/z + \pi\cot\pi z \quad (x<0),\end{aligned} \tag{12}$$

where $n = [x_0] - [x]$. These formulas are used for the computation of $\psi(z)$ in the regions indicated. We have chosen $x_0 = 7$ and $K = 7$.

* An earlier version of this program was written by R. Keyser (CERN).

3. The tests

3.1. *Tests for ln Γ(z)*

The program CLOGAM was checked in the following cases.

(i) The values of $\ln \Gamma(z)$ were computed for $z = x + iy$, where $x = 0(0.5)1(10)$, $y = 0(0.1)10$. The results were compared with the 12-decimal table [23]. Occasional discrepancies of 1 unit in the 12th decimal were found.

(ii) The formula [24]

$$\ln \Gamma(2z) = (2z - 1) \ln 2 + \ln \Gamma(z) + \ln \Gamma(z+\tfrac{1}{2}) - \tfrac{1}{2} \ln \pi , \qquad (13)$$

was "verified" using 500 arguments of the form

$$z = \mu \, [x - \tfrac{1}{2} + i(y - \tfrac{1}{2})] ,$$

where x and y were random numbers uniformly distributed over (0,1). The proportionality factor μ was taken to be $\mu = 2, 5, 10, 30, 50$. For each μ, 100 values z were taken. The two sides of (13) usually agreed to 12–14S (significant digits), occasionally to 11S.

(iii) Calculation $\ln \Gamma(z)$ for $z = x + iy$, where $y = -3.0(0.1)3.0$, $y = \pm 5, \pm 0.01, \pm 0.00001, 0$. This verifies that the imaginary part is computed correctly.

(iv) Computation of $\ln \Gamma(z)$ for

$$z = [(-1)^j x_k + i(-1)^l y_k] \times 10^m ,$$

where $k = 1, 2, 3; j = 2, 3; l = 2, 3; m = 1, 2; x_k = \{0.1, 0.1, 1\}; y_k = \{1, 1, 0.2\}$. The computed values were checked against the values found by direct evaluation of the Stirling series. In particular, for $\mathrm{Re}\, z < 0$, this check is important as an assurance that the sign of the imaginary part of $\ln \Gamma(z)$ is correct.

3.2. *Tests for ψ(z)*

We have tested the following cases using the program CDIGAM.

(i) The formula

$$\psi(2z) = \tfrac{1}{2}[\psi(z) + \psi(z + \tfrac{1}{2})] + \ln 2$$

was checked for the same values of z as formula (13). The two sides agree to 13–14S.

(ii) The relations

$$\mathrm{Im}\, \psi(iy) = 1/2y + \tfrac{1}{2}\pi \coth \pi y ,$$

$$\mathrm{Im}\, \psi(1 + iy) = -1/2y + \tfrac{1}{2}\pi \coth \pi y$$

were checked for $y = 0.1(0.1)1(1)100$. There was agreement to 13–14S.

(iii) Direct evaluation of [24]

$$\psi(z) = \ln z - 1/2z - \int_0^\infty \frac{t \, dt}{(t^2 + z^2)(e^{2\pi t} - 1)} \quad (\mathrm{Re}\, z > 0)$$

for 50 values of z with $0 < \mathrm{Re}\, z \leqslant 10$, $0 < \mathrm{Im}\, z \leqslant 10$. The upper limit of the integral was replaced by $T = (10 \ln 10)/\pi \approx 7.33$. There was agreement to 13–14S.

We note here that relative accuracy is necessarily lost near a zero of $\psi(z)$. These zeros are all negative real, except $x_0 = 1.46163...$. For arguments z with large negative real part $\mathrm{Re}\, z \approx -10^n$, about $(14-n)$ significant digits are correct.

4. Error exits

4.1. *CLOGAM*

If the function subprogram CLOGAM is called with an argument $z = -n \pm i0$, $(n = 0, 1, 2, ...)$ an error message

CLOGAM ... ARGUMENT IS NON-POSITIVE INTEGER

= (n)

is printed on Logical Unit 2, where (n) denotes the argument. The value of CLOGAM is set to zero in this case.

4.2. *CDIGAM*

The function subprogram CDIGAM, when called with an argument $z = -n \pm i0$ $(n = 0, 1, 2, ...)$, prints an error message

CDIGAM ... ARGUMENT IS NON-POSITIVE INTEGER

= (n)

The value of CDIGAM is set to zero in this case.

5. Test run

The results of the test run are self-explanatory.

Acknowledgement

I wish to thank G.A. Erskine for comments and discussions.

Note added in proof

After having sent the manuscript to the editors, the author became aware of a FORTRAN program by Kuki [25], based on a paper by the same author [26]. This program computes the gamma function or its logarithm, for complex arguments, using built-in error control.

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TEST RUN OUTPUT

TEST VALUES FOR LN GAMMA(Z) (Z = X + I*Y)

X	Y	RE LN GAMMA(Z)	IM LN GAMMA(Z)
-13.0	2.0	-26.84992384156715	-37.19840614844497
-9.5	0.0	-12.79589533355426	-31.41592653589794
-3.0	1.0	-2.95350829229571	-9.72641828123693
0.0	8.0	-12.68715285199448	7.83971205351668
3.0	0.0	.69314718055986	0.00000000000000
4.0	2.0	1.25083561935671	2.61019580104885
7.0	4.0	5.41808697187290	7.71810136520472
9.0	16.0	-.27799290829569	39.55316531442281
10.0	0.0	12.80182748008133	0.00000000000000
15.0	5.0	24.34577701569333	13.46736924371726
-13.0	-2.0	-26.84992384156715	37.19840614844497
-9.5	-0.0	-12.79589533355426	31.41592653589794
-3.0	-1.0	-2.95350829229571	9.72641828123693
0.0	-8.0	-12.68715285199448	-7.83971205351668
3.0	-0.0	.69314718055986	-0.00000000000000
4.0	-2.0	1.25083561935671	-2.61019580104885
7.0	-4.0	5.41808697187290	-7.71810136520472
9.0	-16.0	-.27799290829569	-39.55316531442281
10.0	-0.0	12.80182748008133	-0.00000000000000
15.0	-5.0	24.34577701569333	-13.46736924371726

CLOGAM ... ARGUMENT IS NON-POSITIVE INTEGER = -1.00

TEST VALUES FOR PSI(Z) = DIGAMMA(Z)

X	Y	RE PSI(Z)	IM PSI(Z)
-13.0	2.0	2.61375885861489	2.99460095564282
-9.5	0.0	2.30300103429782	0.00000000000000
-3.0	1.0	1.29465032062246	2.87667404746858
0.0	8.0	2.08074567491178	1.63329632679488
3.0	0.0	.92278433509845	0.00000000000000
4.0	2.0	1.39536074614320	.51696112879607
7.0	4.0	2.03269565223019	.55101815665321
9.0	16.0	2.89681672499673	1.08235712929482
10.0	0.0	2.25175258906671	0.00000000000000
15.0	5.0	2.73046382968629	.33195042663378
-13.0	-2.0	2.61375885861489	-2.99460095564282
-9.5	-0.0	2.30300103429782	0.00000000000000
-3.0	-1.0	1.29465032062246	-2.87667404746855
0.0	-8.0	2.08074567491178	-1.63329632679488
3.0	-0.0	.92278433509845	0.00000000000000
4.0	-2.0	1.39536074614320	-.51696112879607
7.0	-4.0	2.03269565223019	-.55101815665321
9.0	-16.0	2.89681672499673	-1.08235712929482
10.0	-0.0	2.25175258906671	0.00000000000000
15.0	-5.0	2.73046382968629	-.33195042663378

CDIGAM ... ARGUMENT IS NON-POSITIVE INTEGER = -1.00