

NAG Library Routine Document

S14ACF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of **bold italicised** terms and other implementation-dependent details.

1 Purpose

S14ACF returns a value of the function $\psi(x) - \ln x$, where ψ is the psi function $\psi(x) = \frac{d}{dx} \ln \Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)}$.

2 Specification

double precision FUNCTION S14ACF(X, IFAIL)

INTEGER IFAIL
double precision X

3 Description

S14ACF returns a value of the function $\psi(x) - \ln x$. The psi function is computed without the logarithmic term so that when x is large, sums or differences of psi functions may be computed without unnecessary loss of precision, by analytically combining the logarithmic terms. For example, the difference $d = \psi(x + \frac{1}{2}) - \psi(x)$ has an asymptotic behaviour for large x given by $d \sim \ln(x + \frac{1}{2}) - \ln x + O(\frac{1}{x^2}) \sim \ln(1 + \frac{1}{2x}) \sim \frac{1}{2x}$.

Computing d directly would amount to subtracting two large numbers which are close to $\ln(x + \frac{1}{2})$ and $\ln x$ to produce a small number close to $\frac{1}{2x}$, resulting in a loss of significant digits. However, using this routine to compute $f(x) = \psi(x) - \ln x$, we can compute $d = f(x + \frac{1}{2}) - f(x) + \ln(1 + \frac{1}{2x})$, and the dominant logarithmic term may be computed accurately from its power series when x is large. Thus we avoid the unnecessary loss of precision.

The routine is derived from the routine PSIFN in Amos (1983).

4 References

Abramowitz M and Stegun I A (1972) *Handbook of Mathematical Functions* (3rd Edition) Dover Publications

Amos D E (1983) Algorithm 610: A portable FORTRAN subroutine for derivatives of the psi function *ACM Trans. Math. Software* **9** 494–502

5 Parameters

- 1: X – **double precision** *Input*
On entry: the argument x of the function.
Constraint: $X > 0.0$.
- 2: IFAIL – INTEGER *Input/Output*
On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.
On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this parameter, the recommended value is 0 . **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry $IFAIL = 0$ or -1 , explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

$IFAIL = 1$

On entry, $X \leq 0.0$. S14ACF returns the value zero.

$IFAIL = 2$

No result is computed because underflow is likely. The value of X is too large. S14ACF returns the value zero.

$IFAIL = 3$

No result is computed because overflow is likely. The value of X is too small. S14ACF returns the value zero.

7 Accuracy

All constants in S14ACF are given to approximately 18 digits of precision. Calling the number of digits of precision in the floating-point arithmetic being used t , then clearly the maximum number of correct digits in the results obtained is limited by $p = \min(t, 18)$.

With the above proviso, results returned by this routine should be accurate almost to full precision, except at points close to the zero of $\psi(x)$, $x \simeq 1.461632$, where only absolute rather than relative accuracy can be obtained.

8 Further Comments

None.

9 Example

The example program reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

9.1 Program Text

```
*      S14ACF Example Program Text
*      Mark 14 Release. NAG Copyright 1989
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
      DOUBLE PRECISION F, X
      INTEGER          IFAIL
*      .. External Functions ..
      DOUBLE PRECISION S14ACF
      EXTERNAL         S14ACF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'S14ACF Example Program Results'
*      Skip heading in data file
      READ (NIN,*)
```

```

      WRITE (NOUT,*)
      WRITE (NOUT,*) '          X          psi(X)-log(X)'
      WRITE (NOUT,*)
20    READ (NIN,*,END=40) X
      IFAIL = 1
*
      F = S14ACF(X,IFAIL)
*
      IF (IFAIL.GE.0) THEN
        WRITE (NOUT,99999) X, F
        GO TO 20
      ELSE
        WRITE (NOUT,99998) IFAIL
      END IF
40    CONTINUE
*
99999 FORMAT (1X,F12.4,F15.4)
99998 FORMAT (1X,' ** S14ACF returned with IFAIL = ',I5)
      END

```

9.2 Program Data

S14ACF Example Program Data
 0.1
 0.5
 3.6
 8.0

9.3 Program Results

S14ACF Example Program Results

X	psi(X)-log(X)
0.1000	-8.1212
0.5000	-1.2704
3.6000	-0.1453
8.0000	-0.0638
