S14ACF – NAG Fortran Library Routine Document

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

```
real FUNCTION S14ACF(X, IFAIL)
INTEGER              IFAIL
real                 X
```

3 Description

This routine 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 $d \sim \ln(x + \frac{1}{2}) - \ln x + O\left(\frac{1}{x^2}\right) \sim \ln\left(1 + \frac{1}{2x}\right) \sim \frac{1}{2x}$.

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 $d = f(x + \frac{1}{2}) - f(x) + \ln\left(1 + \frac{1}{2x}\right)$, 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 [1].

4 References

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

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

5 Parameters

1: X — ***real*** *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. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL $= 0$ unless the routine detects an error (see Section 6).

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 detected by the routine:

IFAIL = 1

On entry, X ≤ 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 subroutine 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 following 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

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S14ACF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             F, X
      INTEGER          IFAIL
*     .. External Functions ..
      real             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 = 0
*
      F = S14ACF(X,IFAIL)
*
      WRITE (NOUT,99999) X, F
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,F12.4,F15.4)
      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
```