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 $\psi(x) = \dfrac{d}{dx} \ln \Gamma(x) = \dfrac{\Gamma'(x)}{\Gamma(x)}$.

2   Specification

```
FUNCTION S14ACF (X, IFAIL)
REAL (KIND=nag_wp) S14ACF

INTEGER           IFAIL
REAL (KIND=nag_wp) 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 $d = \psi\left(x + \frac{1}{2}\right) - \psi(x)$ has an asymptotic behaviour for large x given by

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

Computing d directly would amount to subtracting two large numbers which are close to $\ln\left(x + \frac{1}{2}\right)$ 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 $d = f\left(x + \frac{1}{2}\right) - f(x) + \ln\left(1 + \frac{1}{2x}\right)$, 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 (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 – REAL (KIND=nag_wp)   *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.

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.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (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 or warnings 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.

IFAIL = −99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.8 in the Essential Introduction for further information.

IFAIL = −399

Your licence key may have expired or may not have been installed correctly.

See Section 3.7 in the Essential Introduction for further information.

IFAIL = −999

Dynamic memory allocation failed.

See Section 3.6 in the Essential Introduction for further information.

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 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 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.

10.1 Program Text

```
      Program s14acfe

!     S14ACF Example Program Text

!     Mark 25 Release. NAG Copyright 2014.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, s14acf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: f, x
      Integer                          :: ifail, ioerr
!     .. 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,*)

data: Do
        Read (nin,*,Iostat=ioerr) x

        If (ioerr<0) Then
          Exit data
        End If

        ifail = -1
        f = s14acf(x,ifail)

        If (ifail<0) Then
          Exit data
        End If

        Write (nout,99999) x, f
      End Do data

99999 Format (1X,F12.4,F15.4)
      End Program s14acfe
```

10.2 Program Data

```
S14ACF Example Program Data
0.1
0.5
3.6
8.0
```
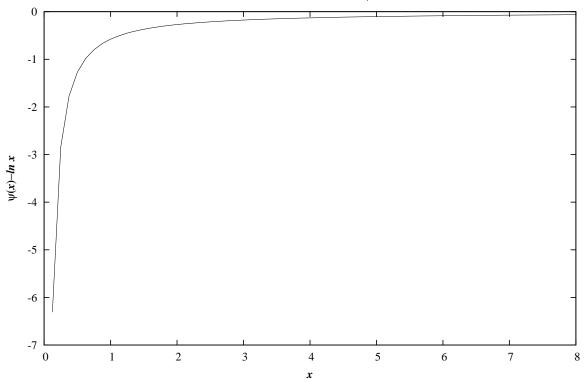
10.3 Program Results

```
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
```

Example Program
Returns a Value of the Function $\psi(x) - \ln x$