NAG Fortran Library Routine Document

S14AEF

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

S14AEF returns the value of the kth derivative of the psi function $\psi(x)$ for real x and $k = 0, 1, \ldots, 6$, via the routine name.

2 Specification

```
real FUNCTION S14AEF(X, K, IFAIL)
INTEGER              K, IFAIL
real                 X
```

3 Description

This routine evaluates an approximation to the kth derivative of the psi function $\psi(x)$ given by

$$\psi^{(k)}(x) = \frac{d^k}{dx^k}\psi(x) = \frac{d^k}{dx^k}\left(\frac{d}{dx}\log_{\mathrm{e}}\Gamma(x)\right),$$

where x is real with $x \neq 0, -1, -2, \ldots$ and $k = 0, 1, \ldots, 6$. For negative non-integer values of x, the recurrence relationship

$$\psi^{(k)}(x+1) = \psi^{(k)}(x) + \frac{d^k}{dx^k}\left(\frac{1}{x}\right)$$

is used. The value of $\dfrac{(-1)^{k+1}\psi^{(k)}(x)}{k!}$ is obtained by a call to S14ADF, which is based on the routine PSIFN in Amos (1983).

Note that $\psi^{(k)}(x)$ is also known as the *polygamma* function. Specifically, $\psi^{(0)}(x)$ is often referred to as the *digamma* function and $\psi^{(1)}(x)$ as the *trigamma* function in the literature. Further details can be found in Abramowitz and Stegun (1972).

4 References

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

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

5 Parameters

1: X – ***real*** *Input*

On entry: the argument x of the function.

Constraint: X must not be 'too close' (see Section 6) to a non-positive integer.

2: K – INTEGER *Input*

On entry: the function $\psi^{(k)}(x)$ to be evaluated.

Constraint: $0 \leq \mathrm{K} \leq 6$.

3: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 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, for users 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, K < 0,
or K > 6,
or X is 'too close' to a non-positive integer. That is, ABS(X $-$ NINT(X)) $<$ ***machine precision*** $\times$ NINT(ABS(X)).

IFAIL $= 2$

The evaluation has been abandoned due to the likelihood of underflow. The result is returned as zero.

IFAIL $= 3$

The evaluation has been abandoned due to the likelihood of overflow. The result is returned as zero.

7 Accuracy

All constants in routine S14ADF are given to approximately 18 digits of precision. If t denotes the number of digits of precision in the floating-point arithmetic being used, then clearly the maximum number in the results obtained is limited by $p = \min(t, 18)$. Empirical tests by Amos (1983) have shown that the maximum relative error is a loss of approximately two decimal places of precision. Further tests with the function $-\psi^{(0)}(x)$ have shown somewhat improved accuracy, except at points near the positive zero of $\psi^{(0)}(x)$ at $x = 1.46\ldots$, where only absolute accuracy can be obtained.

8 Further Comments

None.

9 Example

The example program evaluates $\psi^{(2)}(x)$ at $x = 2.5$, 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.

```
*     S14AEF Example Program Text.
*     Mark 20 Release. NAG Copyright 2001.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL, K
*     .. External Functions ..
      real             S14AEF
      EXTERNAL         S14AEF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14AEF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '   X     K    (D^K/DX^K)psi(X)    IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X, K
      IFAIL = 0
*
      Y = S14AEF(X,K,IFAIL)
*
      WRITE (NOUT,99999) X, K, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,F5.1,I5,5X,1P,E12.4,3X,I7)
      END
```

9.2 Program Data

```
S14AEF Example Program Data
 2.5   2  : Values of X and K
```

9.3 Program Results

```
 S14AEF Example Program Results

    X     K    (D^K/DX^K)psi(X)    IFAIL

   2.5    2      -2.3620E-01         0
```