NAG 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

double precision `FUNCTION S14AEF(X, K, IFAIL)`
`INTEGER` `K, IFAIL`
double precision `X`

3 Description

S14AEF 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 noninteger 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

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 must not be 'too close' (see Section 6) to a nonpositive 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. 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, K < 0,
or K > 6,
or X is 'too close' to a nonpositive 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 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

This example evaluates $\psi^{(2)}(x)$ at $x = 2.5$, and prints the results.

9.1 Program Text

```
*     S14AEF Example Program Text
*     Mark 20 Release. NAG Copyright 2001.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      DOUBLE PRECISION X, Y
      INTEGER          IFAIL, K
*     .. External Functions ..
      DOUBLE PRECISION 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 = 1
*
      Y = S14AEF(X,K,IFAIL)
*
      IF (IFAIL.GE.0) THEN
         WRITE (NOUT,99999) X, K, Y, IFAIL
         GO TO 20
      ELSE
         WRITE (NOUT,99998) IFAIL
      END IF
   40 CONTINUE
*
99999 FORMAT (1X,F5.1,I5,5X,1P,E12.4,3X,I7)
99998 FORMAT (1X,' ** S14AEF returned with IFAIL = ',I5)
      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
```