

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 k th derivative of the psi function $\psi(x)$ for real x and $k = 0, 1, \dots, 6$, 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 k th derivative of the psi function $\psi(x)$ given by

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

where x is real with $x \neq 0, -1, -2, \dots$ and $k = 0, 1, \dots, 6$. 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 $\frac{(-1)^{k+1} \psi^{(k)}(x)}{k!}$ 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: $0 \leq K \leq 6$.

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, $\text{abs}(X - \text{nint}(X)) < \text{machine precision} \times \text{nint}(\text{abs}(X))$.

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 $x = 1.46\dots$, 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
