NAG Fortran Library Routine Document

S14ADF

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

S14ADF returns a sequence of values of scaled derivatives of the psi function $\psi(x)$.

2 Specification

```
SUBROUTINE S14ADF(X, N, M, ANS, IFAIL)
INTEGER           N, M, IFAIL
real              X, ANS(M)
```

3 Description

This routine computes m values of the function

$$w(k,x) = \frac{(-1)^{k+1}\psi^{(k)}(x)}{k!},$$

for $x > 0$, $k = n,\ n+1,\ldots,n+m-1$, where ψ is the psi function

$$\psi(x) = \frac{d}{dx}\ln\Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)},$$

and $\psi^{(k)}$ denotes the kth derivative of ψ.

The routine is derived from the routine PSIFN in Amos (1983). The basic method of evaluation of $w(k,x)$ is the asymptotic series

$$w(k,x) \sim \epsilon(k,x) + \frac{1}{2x^{k+1}} + \frac{1}{x^k}\sum_{j=1}^{\infty} B_{2j}\frac{(2j+k-1)!}{(2j)!\,k!\,x^{2j}}$$

for large x greater than a machine-dependent value x_{min}, followed by backward recurrence using

$$w(k,x) = w(k,x+1) + x^{-k-1}$$

for smaller values of x, where $\epsilon(k,x) = -\ln x$ when $k = 0$, $\epsilon(k,x) = \dfrac{1}{kx^k}$ when $k > 0$, and B_{2j}, $j = 1,2,\ldots,$ are the Bernoulli numbers.

When k is large, the above procedure may be inefficient, and the expansion

$$w(k,x) = \sum_{j=1}^{\infty}\frac{1}{(x+j)^{k+1}},$$

which converges rapidly for large k, is used instead.

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 > 0.0.

2: N – INTEGER *Input*

On entry: the index of the first member n of the sequence of functions.

Constraint: N ≥ 0.

3: M – INTEGER *Input*

On entry: the number of members m required in the sequence $w(k, x)$, for $k = n, n+1, \ldots, n+m-1$.

Constraint: M ≥ 1.

4: ANS(M) – ***real*** array *Output*

On exit: the first m elements of ANS contain the required values $w(k, x)$, for $k = n, n+1, \ldots, n+m-1$.

5: 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, X ≤ 0.0.

IFAIL $= 2$

On entry, N < 0.

IFAIL $= 3$

On entry, M < 1.

IFAIL $= 4$

No results are returned because underflow is likely. Either X or N + M − 1 is too large. If possible, reduce the value of M and call S14ADF again.

IFAIL $= 5$

No results are returned because overflow is likely. Either X is too small, or N + M − 1 is too large. If possible, reduce the value of M and call S14ADF again.

IFAIL = 6

No results are returned because there is not enough internal workspace to continue computation. N + M − 1 may be too large. If possible, reduce the value of M and call S14ADF again.

7 Accuracy

All constants in subroutine S14ADF 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 $p = \min(t, 18)$. Empirical tests of S14ADF, taking values of x in the range $0.0 < x < 50.0$, and n in the range $1 \leq n \leq 50$, have shown that the maximum relative error is a loss of approximately two decimal places of precision. Tests with $n = 0$, i.e., testing the function $-\psi(x)$, have shown somewhat better accuracy, except at points close to the zero of $\psi(x)$, $x \simeq 1.461632$, where only absolute accuracy can be obtained.

8 Further Comments

The time taken for a call of S14ADF is approximately proportional to m, plus a constant. In general, it is much cheaper to call S14ADF with m greater than 1 to evaluate the function $w(k,x)$, for $k = n, n+1, \ldots, n+m-1$, rather than to make m separate calls of S14ADF.

9 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.

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.

```
*     S14ADF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX
      PARAMETER        (MMAX=4)
*     .. Local Scalars ..
      real             X
      INTEGER          I, IFAIL, M, N
*     .. Local Arrays ..
      real             W(MMAX)
*     .. External Subroutines ..
      EXTERNAL         S14ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
     +'      X           W(1)          W(2)          W(3)          W(4)'
      WRITE (NOUT,*)
      N = 0
      M = 4
   20 READ (NIN,*,END=40) X
*
      CALL S14ADF(X,N,M,W,IFAIL)
*
      WRITE (NOUT,99999) X, (W(I),I=1,M)
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,5(e12.4,2X))
```

```
      END
```

9.2 Program Data

```
S14ADF Example Program Data
0.1
0.5
3.6
8.0
```

9.3 Program Results

```
 S14ADF Example Program Results

       X            W(1)          W(2)          W(3)          W(4)

   1.0000E-01    1.0424E+01    1.0143E+02    1.0009E+03    1.0001E+04
   5.0000E-01    1.9635E+00    4.9348E+00    8.4144E+00    1.6235E+01
   3.6000E+00   -1.1357E+00    3.1988E-01    5.0750E-02    1.0653E-02
   8.0000E+00   -2.0156E+00    1.3314E-01    8.8498E-03    7.8321E-04
```