

NAG 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 $\psi(x)$ (also known as the digamma function).

2 Specification

SUBROUTINE S14ADF(X, N, M, ANS, IFAIL)

INTEGER N, M, IFAIL

double precision X, ANS(M)

3 Description

S14ADF computes m values of the function

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

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

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

and $\psi^{(k)}$ denotes the k th 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 $k = 0$, $\epsilon(k, x) = \frac{1}{kx^k}$ when $k > 0$, and B_{2j} , $j = 1, 2, \dots$, 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

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: $X > 0.0$.
- 2: N – INTEGER *Input*
On entry: the index of the first member n of the sequence of functions.
Constraint: $N \geq 0$.
- 3: M – INTEGER *Input*
On entry: the number of members m required in the sequence $w(k, x)$, for $k = n, n + 1, \dots, n + m - 1$.
Constraint: $M \geq 1$.
- 4: $ANS(M)$ – *double precision* array *Output*
On exit: the first m elements of ANS contain the required values $w(k, x)$, for $k = n, n + 1, \dots, n + m - 1$.
- 5: $IFAIL$ – 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, $X \leq 0.0$.

$IFAIL = 2$

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 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 $k = n, n + 1, \dots, n + m - 1$, rather than to make m separate calls of S14ADF.

9 Example

This example 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

```
*      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 ..
      DOUBLE PRECISION X
      INTEGER          I, IFAIL, M, N
*      .. Local Arrays ..
      DOUBLE PRECISION ANS(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          ANS(1)          ANS(2)          ',
+ 'ANS(3)          ANS(4)'
      WRITE (NOUT,*)
      N = 0
      M = 4
20 READ (NIN,*,END=40) X
*
      IFAIL = 1
      CALL S14ADF(X,N,M,ANS,IFAIL)
*
      IF (IFAIL.GE.0) THEN
        WRITE (NOUT,99999) X, (ANS(I),I=1,M)
        GO TO 20
      ELSE
        WRITE (NOUT,99998) IFAIL
      END IF
```

```

      40 CONTINUE
*
99999 FORMAT (1X,1P,5(E12.4,2X))
99998 FORMAT (1X,' ** S14ADF returned with IFAIL = ',I5)
      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	ANS(1)	ANS(2)	ANS(3)	ANS(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
