S15ADF – NAG Fortran Library Routine Document

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

S15ADF returns the value of the complementary error function, $\mathrm{erfc}\, x$, via the routine name.

2 Specification

```
real FUNCTION S15ADF(X, IFAIL)
INTEGER              IFAIL
real                 X
```

3 Description

The routine calculates an approximate value for the complement of the error function

$$\mathrm{erfc}\, x = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du = 1 - \mathrm{erf}\, x.$$

For $x \geq 0$, it is based on the Chebyshev expansion

$$\mathrm{erfc}\, x = e^{-x^2} y(x),$$

where $y(x) = {\sum_{r=0}}' a_r T_r(t)$ and $t = (x - 3.75)/(x + 3.75)$, $-1 \leq t \leq +1$.

For $x \geq x_{hi}$, where there is a danger of setting underflow, the result is returned as zero.

For $x < 0$, $\mathrm{erfc}\, x = 2 - e^{-x^2} y(|x|)$.

For $x < x_{low} < 0$, the result is returned as 2.0 which is correct to within ***machine precision***. The values of x_{hi} and x_{low} are given in the Users' Note for your implementation.

4 References

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

5 Parameters

1: X — ***real*** *Input*

On entry: the argument x of the function.

2: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors detected by the routine:

There are no failure exits from this routine. The parameter IFAIL has been included for consistency with other routines in this chapter.

7 Accuracy

If δ and ϵ are relative errors in the argument and result, respectively, then in principle

$$|\epsilon| \simeq \left| \frac{2xe^{-x^2}}{\sqrt{\pi}\,\mathrm{erfc}\,x}\delta \right|.$$

That is, the relative error in the argument, x, is amplified by a factor $\frac{2xe^{-x^2}}{\sqrt{\pi}\,\mathrm{erfc}\,x}$ in the result.

The behaviour of this factor is shown in Figure 1.

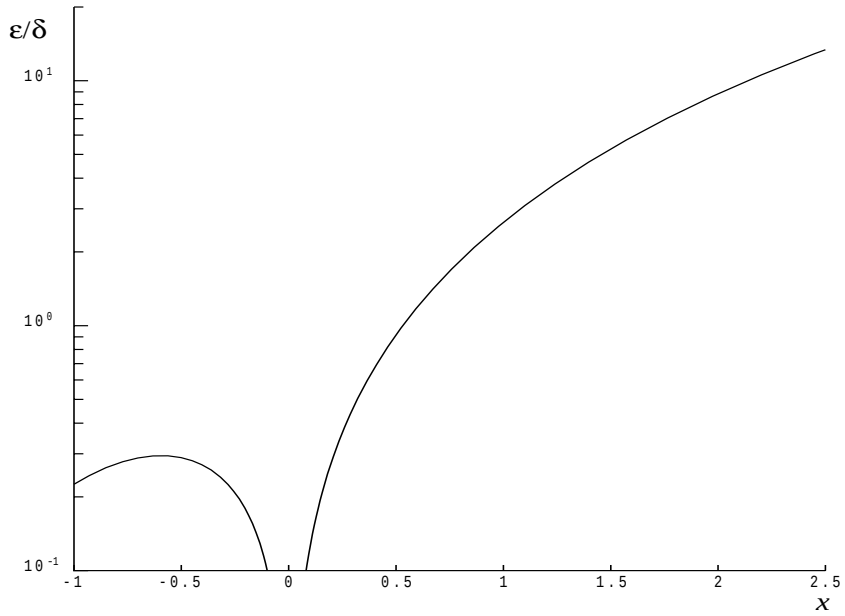

Figure 1

It should be noted that near $x = 0$ this factor behaves as $\frac{2x}{\sqrt{\pi}}$ and hence the accuracy is largely determined by the ***machine precision***. Also for large negative x, where the factor is $\sim \frac{xe^{-x^2}}{\sqrt{\pi}}$, accuracy is mainly limited by ***machine precision***. However, for large positive x, the factor becomes $\sim 2x^2$ and to an extent relative accuracy is necessarily lost. The absolute accuracy E is given by

$$E \simeq \frac{2xe^{-x^2}}{\sqrt{\pi}}\delta$$

so absolute accuracy is guaranteed for all x.

8 Further Comments

None.

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.

```
*     S15ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15ADF
      EXTERNAL         S15ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S15ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2 Program Data

```
S15ADF Example Program Data
          -10.0
           -1.0
            0.0
            1.0
           10.0
```

9.3 Program Results

```
 S15ADF Example Program Results

      X           Y        IFAIL

  -1.000E+01   2.000E+00      0
  -1.000E+00   1.843E+00      0
   0.000E+00   1.000E+00      0
   1.000E+00   1.573E-01      0
   1.000E+01   2.088E-45      0
```