NAG Fortran Library Routine Document

S15ADF

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, 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

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

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

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

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 $x < 0$, 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

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.

2:    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

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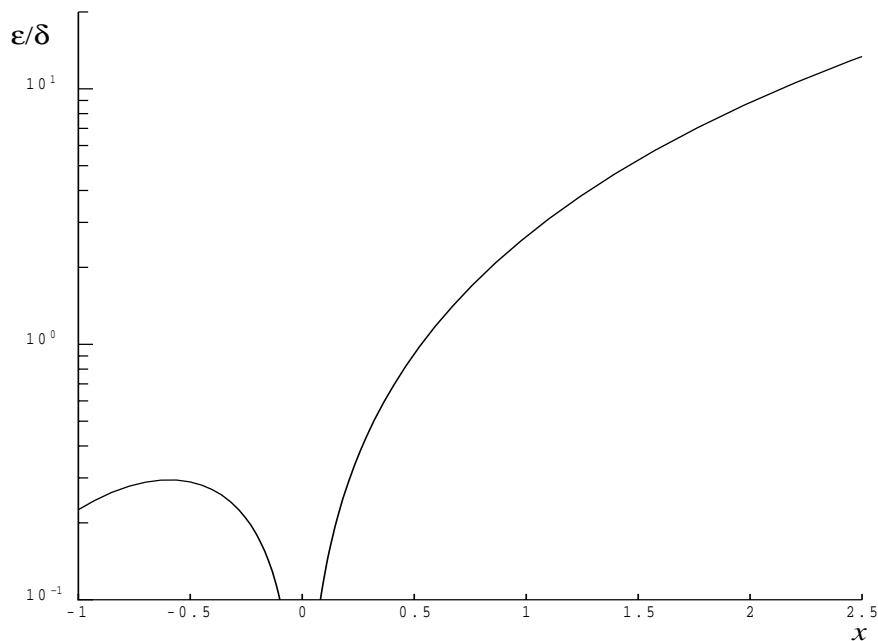
7   Accuracy

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 $\dfrac{2xe^{-x^2}}{\sqrt{\pi}\,\mathrm{erfc}\,x}$ 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 $\sim \dfrac{xe^{-x^2}}{\sqrt{\pi}}$, 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
```