NAG 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, $\mathrm{erfc}(x)$, via the routine name.

2 Specification

```
double precision FUNCTION S15ADF(X, IFAIL)
INTEGER                         IFAIL
double precision                X
```

3 Description

S15ADF calculates an approximate value for the complement of the error function

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2}\, dt = 1 - \mathrm{erf}(x).$$

Let $\hat{x}$ be the root of the equation $\mathrm{erfc}(x) - \mathrm{erf}(x) = 0$ (then $\hat{x} \approx 0.46875$). For $|x| \leq \hat{x}$ the value of $\mathrm{erfc}(x)$ is based on the following rational Chebyshev expansion for $\mathrm{erf}(x)$:

$$\mathrm{erf}(x) \approx x R_{\ell,m}\left(x^2\right),$$

where $R_{\ell,m}$ denotes a rational function of degree ℓ in the numerator and m in the denominator.

For $|x| > \hat{x}$ the value of $\mathrm{erfc}(x)$ is based on a rational Chebyshev expansion for $\mathrm{erfc}(x)$: for $\hat{x} < |x| \leq 4$ the value is based on the expansion

$$\mathrm{erfc}(x) \approx e^{x^2} R_{\ell,m}(x);$$

and for $|x| > 4$ it is based on the expansion

$$\mathrm{erfc}(x) \approx \frac{e^{x^2}}{x} \left(\frac{1}{\sqrt{\pi}} + \frac{1}{x^2} R_{\ell,m}\left(1/x^2\right) \right).$$

For each expansion, the specific values of ℓ and m are selected to be minimal such that the maximum relative error in the expansion is of the order 10^{-d}, where d is the maximum number of decimal digits that can be accurately represented for the particular implementation (see X02BEF).

For $|x| \geq x_{\mathrm{hi}}$ there is a danger of setting underflow in $\mathrm{erfc}(x)$ (the value of x_{hi} is given in the Users' Note for your implementation). For $x \geq x_{\mathrm{hi}}$, S15ADF returns $\mathrm{erfc}(x) = 0$; for $x \leq -x_{\mathrm{hi}}$ it returns $\mathrm{erfc}(x) = 2$.

4 References

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

Cody W J (1969) Rational Chebyshev Approximations for the Error Function *Math.Comp.* **23** 631–637

5 Parameters

1: X – ***double precision*** *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. 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

There are no failure exits from S15ADF. 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.

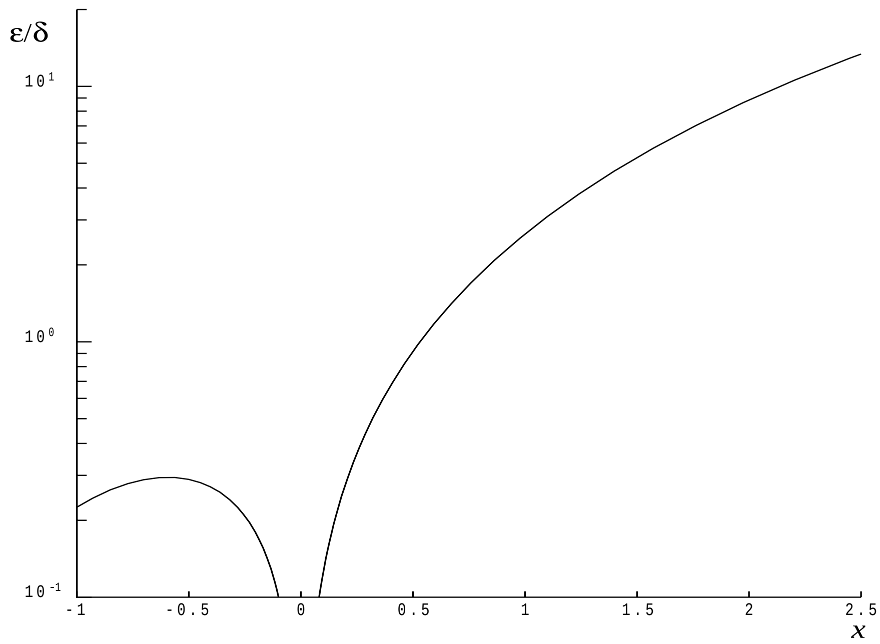

Figure 1

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

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

```
*     S15ADF Example Program Text
*     Mark 14 Revised. NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      DOUBLE PRECISION X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      DOUBLE PRECISION 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)
*
      IF (IFAIL.GE.0) THEN
         WRITE (NOUT,99999) X, Y, IFAIL
         GO TO 20
      ELSE
         WRITE (NOUT,99998) IFAIL
      END IF
   40 CONTINUE
*
99999 FORMAT (1X,1P,2E12.3,I7)
99998 FORMAT (1X,' ** S15ADF returned with IFAIL = ',I5)
      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
```