

NAG Library Routine Document

S15AEF

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

S15AEF returns the value of the error function $\operatorname{erf}(x)$, via the routine name.

2 Specification

double precision FUNCTION S15AEF(X, IFAIL)
 INTEGER IFAIL
double precision X

3 Description

S15AEF calculates an approximate value for the error function

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt = 1 - \operatorname{erfc}(x).$$

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

$$\operatorname{erf}(x) \approx xR_{\ell,m}(x^2),$$

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

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

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

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

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 $|x| \geq x_{\text{hi}}$ there is a danger of setting underflow in $\operatorname{erfc}(x)$ (the value of x_{hi} is given in the Users' Note for your implementation). For $x \geq x_{\text{hi}}$, S15AEF returns $\operatorname{erf}(x) = 1$; for $x \leq -x_{\text{hi}}$ it returns $\operatorname{erf}(x) = -1$.

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 S15AEF. The parameter IFAIL has been included for consistency with other routines in this chapter.

7 Accuracy

See Section 7 in S15ADF.

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

```
*      S15AEF 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 S15AEF
      EXTERNAL         S15AEF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'S15AEF 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 = S15AEF(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,' ** S15AEF returned with IFAIL = ',I5)
END
```

9.2 Program Data

```
S15AEF Example Program Data
      -6.0
      -4.5
      -1.0
       1.0
       4.5
       6.0
```

9.3 Program Results

```
S15AEF Example Program Results
```

X	Y	IFAIL
-6.000E+00	-1.000E+00	0
-4.500E+00	-1.000E+00	0
-1.000E+00	-8.427E-01	0
1.000E+00	8.427E-01	0
4.500E+00	1.000E+00	0
6.000E+00	1.000E+00	0
