NAG Library Routine Document

S15AGF

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

S15AGF returns the value of the scaled complementary error function $\mathrm{erfcx}(x)$, via the routine name.

2 Specification

double precision `FUNCTION S15AGF(X, IFAIL)`

```
INTEGER                  IFAIL
double precision         X
```

3 Description

S15AGF calculates an approximate value for the scaled complementary error function

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

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 $\mathrm{erfcx}(x)$ is based on the following rational Chebyshev expansion for $\mathrm{erf}(x)$:

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

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 $\mathrm{erfcx}(x)$ 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).

Asymptotically, $\mathrm{erfcx}(x) \sim 1/\left(\sqrt{\pi}\,\mathrm{abs}(x)\right)$. There is a danger of setting underflow in $\mathrm{erfcx}(x)$ whenever $x \geq x_{\mathrm{hi}} = \min\left(x_{\mathrm{huge}}, 1/\left(\sqrt{\pi}x_{\mathrm{tiny}}\right)\right)$, where x_{huge} is the largest positive model number (see X02ALF) and x_{tiny} is the smallest positive model number (see X02AKF). In this case S15AGF exits with IFAIL $= 1$ and returns $\mathrm{erfcx}(x) = 0$. For x in the range $1/\left(2\sqrt{\epsilon}\right) \leq x < x_{\mathrm{hi}}$, where ϵ is the ***machine precision***, the asymptotic value $1/\left(\sqrt{\pi}\,\mathrm{abs}(x)\right)$ is returned for $\mathrm{erfcx}(x)$ and S15AGF exits with IFAIL $= 2$.

There is a danger of setting overflow in e^{x^2} whenever $x < x_{\mathrm{neg}} = -\sqrt{\log\left(x_{\mathrm{huge}}/2\right)}$. In this case S15AGF exits with IFAIL $= 3$ and returns $\mathrm{erfcx}(x) = x_{\mathrm{huge}}$.

The values of x_{hi}, $1/\left(2\sqrt{\epsilon}\right)$ and x_{neg} 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

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, because for this routine the values of the output parameters may be useful even if IFAIL $\neq 0$ on exit, the recommended value is -1. **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).

Note: S15AGF may return useful information for one or more of the following detected errors or warnings.

Errors or warnings detected by the routine:

IFAIL $= 1$

On entry, X $\geq x_{\mathrm{hi}}$ (see Section 3). On soft failure the function value returned is 0.

IFAIL $= 2$

On entry, $1/\left(2\sqrt{\epsilon}\right) \leq$ X $< x_{\mathrm{hi}}$ (see Section 3). On soft failure the function value returned is $1/\left(\sqrt{\pi}\,\mathrm{abs(X)}\right)$.

IFAIL $= 3$

On entry, X $< x_{\mathrm{neg}}$ (see Section 3). On soft failure the function value returned is the largest positive model number.

7 Accuracy

The relative error in computing $\mathrm{erfcx}(x)$ may be estimated by evaluating

$$E = \frac{\mathrm{erfcx}(x) - e^{x^2}\sum_{n=1}^{\infty} I^n\,\mathrm{erfc}(x)}{\mathrm{erfcx}(x)},$$

where I^n denotes repeated integration. Empirical results suggest that on the interval $(\hat{x}, 2)$ the loss in base b significant digits for maximum relative error is around 3.3, while for root-mean-square relative error on that interval it is 1.2 (see X02BHF for the definition of the model parameter b). On the interval $(2, 20)$ the values are around 3.5 for maximum and 0.45 for root-mean-square relative errors; note that on these two intervals $\mathrm{erfc}(x)$ is the primary computation. See also 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

```
*     S15AGF Example Program Text
*     Mark 22 Release. NAG Copyright 2007.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      DOUBLE PRECISION X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      DOUBLE PRECISION S15AGF
      EXTERNAL         S15AGF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15AGF Example Program Results'
*
*     Skip heading in data file
*
      READ (NIN,*)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) '       X          ERFCX(X)    IFAIL'
      WRITE (NOUT,*)
*
   20 CONTINUE
*
      READ (NIN,*,END=40) X
*
      IFAIL = 1
*
      Y = S15AGF(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,2(1X,E13.5),1X,I3)
99998 FORMAT (1X,' ** S15AGF returned with IFAIL = ',I5)
      END
```

9.2 Program Data

```
S15AGF Example Program Data
           -30.0
           -6.0
           -4.5
           -1.0
            1.0
            4.5
            6.0
            7.0D7
```

9.3 Program Results

```
 S15AGF Example Program Results

        X          ERFCX(X)    IFAIL

   -3.00000E+01   1.79769+308   3
   -6.00000E+00   8.62246E+15   0
   -4.50000E+00   1.24593E+09   0
   -1.00000E+00   5.00898E+00   0
    1.00000E+00   4.27584E-01   0
    4.50000E+00   1.22485E-01   0
    6.00000E+00   9.27766E-02   0
    7.00000E+07   8.05985E-09   2
```