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 erfcx(x), via the function name.

2 Specification

```
FUNCTION S15AGF (X, IFAIL)
REAL (KIND=nag_wp) S15AGF
INTEGER            IFAIL
REAL (KIND=nag_wp) X
```

3 Description

S15AGF calculates an approximate value for the scaled complementary error function

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

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

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

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

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

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

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

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, erfcx$(x) \sim 1/(\sqrt{\pi}|x|)$. There is a danger of setting underflow in erfcx(x) whenever $x \geq x_{\text{hi}} = \min\left(x_{\text{huge}}, 1/\left(\sqrt{\pi}x_{\text{tiny}}\right)\right)$, 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 erfcx$(x) = 0$. For x in the range $1/(2\sqrt{\epsilon}) \leq x < x_{\text{hi}}$, where ϵ is the ***machine precision***, the asymptotic value $1/(\sqrt{\pi}|x|)$ is returned for erfcx(x) and S15AGF exits with IFAIL $= 2$.

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

The values of x_{hi}, $1/(2\sqrt{\epsilon})$ 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 Arguments

1: X – REAL (KIND=nag_wp) *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 argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

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 arguments 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.**

On exit: IFAIL $= 0$ unless the routine detects an error or a warning has been flagged (see Section 6).

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 $= \langle value \rangle$ and the constant $x_{\mathrm{hi}} = \langle value \rangle$.
Constraint: X $< x_{\mathrm{hi}}$.

IFAIL $= 2$

On entry, |X| was in the interval $[\langle value \rangle, \langle value \rangle)$ where erfcx(X) is approximately $1/(\sqrt{\pi} * |\mathrm{X}|)$: X $= \langle value \rangle$.

IFAIL $= 3$

On entry, X $= \langle value \rangle$ and the constant $x_{\mathrm{neg}} = \langle value \rangle$.
Constraint: X $\geq x_{\mathrm{neg}}$.

IFAIL $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -399$

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -999$

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

The relative error in computing erfcx(x) may be estimated by evaluating

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

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 erfc(x) is the primary computation. See also Section 7 in S15ADF.

8 Parallelism and Performance

S15AGF is not threaded in any implementation.

9 Further Comments

None.

10 Example

This example reads values of the argument x from a file, evaluates the function at each value of x and prints the results.

10.1 Program Text

```
    Program s15agfe

!     S15AGF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, s15agf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: x, y
      Integer                          :: ifail, ioerr
!     .. Executable Statements ..
      Write (nout,*) 'S15AGF Example Program Results'

!     Skip heading in data file
      Read (nin,*)

      Write (nout,*)
      Write (nout,*) '       X          erfcx(X)'
      Write (nout,*)

data: Do
        Read (nin,*,Iostat=ioerr) x

        If (ioerr<0) Then
```

```
          Exit data
        End If

        ifail = -1
        y = s15agf(x,ifail)

        If (ifail<0) Then
          Exit data
        End If

        Write (nout,99999) x, y
      End Do data

99999 Format (1X,1P,2(1X,E13.5))
    End Program s15agfe
```

10.2 Program Data

```
S15AGF Example Program Data
           -6.0
           -4.5
           -1.0
            1.0
            4.5
            6.0
```

10.3 Program Results

```
 S15AGF Example Program Results

        X          erfcx(X)

   -6.00000E+00   8.62246E+15
   -4.50000E+00   1.24593E+09
   -1.00000E+00   5.00898E+00
    1.00000E+00   4.27584E-01
    4.50000E+00   1.22485E-01
    6.00000E+00   9.27766E-02
```