

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, $\text{erfc}(x)$, via the function name.

2 Specification

```
FUNCTION S15ADF (X, IFAIL)
REAL (KIND=nag_wp) S15ADF
INTEGER IFAIL
REAL (KIND=nag_wp) X
```

3 Description

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

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

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

$$\text{erf}(x) \approx x R_{\ell,m}(x^2),$$

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 $\text{erfc}(x)$ is based on a rational Chebyshev expansion for $\text{erfc}(x)$: 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

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

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

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 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, if you are not familiar with this argument, the recommended value is 0. **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

There are no failure exits from S15ADF. The argument 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

$$|\epsilon| \simeq \left| \frac{2xe^{-x^2}}{\sqrt{\pi} \operatorname{erfc}(x)} \delta \right|.$$

That is, the relative error in the argument, x , is amplified by a factor $\frac{2xe^{-x^2}}{\sqrt{\pi} \operatorname{erfc}(x)}$ in the result.

The behaviour of this factor is shown in Figure 1.

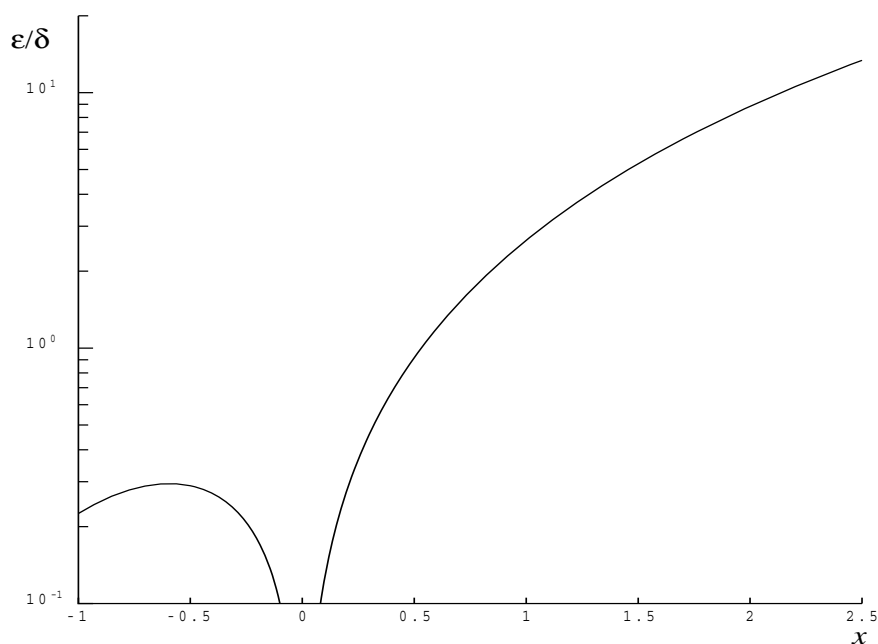


Figure 1

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 Parallelism and Performance

S15ADF 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 s15adfe

!      S15ADF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
      Use nag_library, Only: nag_wp, s15adf
!      .. 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,*) 'S15ADF Example Program Results'

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

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

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

      If (ioerr<0) Then
         Exit data
      End If

      ifail = 0
      y = s15adf(x,ifail)

```

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

99999 Format (1X,1P,2E12.3)
End Program s15adfe
```

10.2 Program Data

```
S15ADF Example Program Data
      -10.0
      -1.0
       0.0
       1.0
      10.0
```

10.3 Program Results

S15ADF Example Program Results

X	Y
-1.000E+01	2.000E+00
-1.000E+00	1.843E+00
0.000E+00	1.000E+00
1.000E+00	1.573E-01
1.000E+01	2.088E-45
