S15AFF – NAG Fortran Library Routine Document

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

S15AFF returns a value for Dawson's Integral, $F(x)$, via the routine name.

2 Specification

```
real FUNCTION S15AFF(X, IFAIL)
INTEGER              IFAIL
real                 X
```

3 Description

This routine evaluates an approximation for Dawson's Integral

$$F(x) = e^{-x^2} \int_0^x e^{t^2}\, dt.$$

The routine is based on two Chebyshev expansions:

For $0 < |x| \leq 4$,

$$F(x) = x {\sum_{r=0}}' a_r T_r(t), \qquad \text{where } t = 2\left(\frac{x}{4}\right)^2 - 1.$$

For $|x| > 4$,

$$F(x) = \frac{1}{x} {\sum_{r=0}}' b_r T_r(t), \qquad \text{where } t = 2\left(\frac{4}{x}\right)^2 - 1.$$

For $|x|$ near zero, $F(x) \simeq x$, and for $|x|$ large, $F(x) \simeq \frac{1}{2x}$. These approximations are used for those values of x for which the result is correct to ***machine precision***. For very large x on some machines, $F(x)$ may underflow and then the result is set exactly to zero (see the Users' Note for your implementation for details).

4 References

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

5 Parameters

1: X — ***real*** *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. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors detected by the routine:

There are no error exits from this routine. The parameter IFAIL is included for consistency with other routines in this chapter.

7 Accuracy

Let δ and ϵ be the relative errors in the argument and result respectively.

If δ is considerably greater than the ***machine precision*** (i.e., if δ is due to data errors etc.), then ϵ and δ are approximately related by:

$$\epsilon \simeq \left| \frac{x(1-2xF(x))}{F(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor $\left| \frac{x(1-2xF(x))}{F(x)} \right|$:

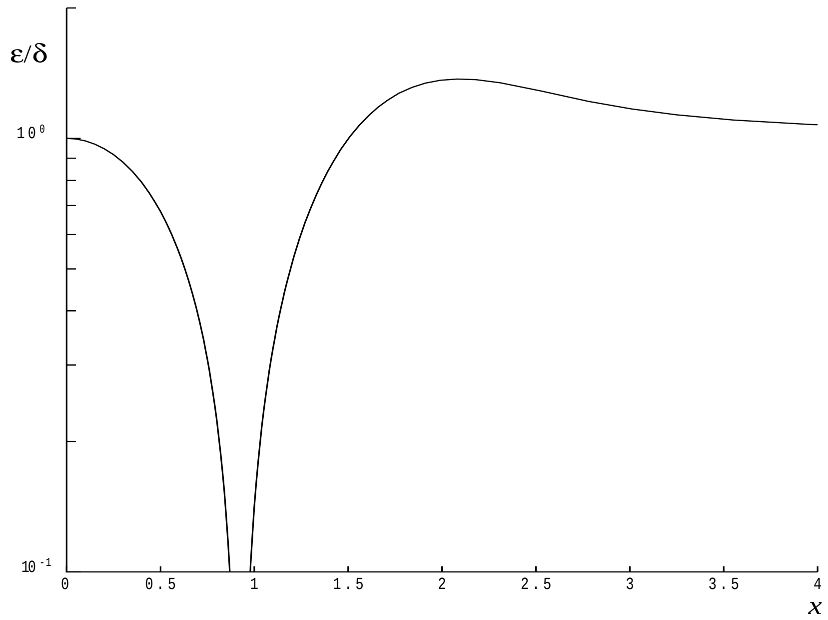

Figure 1

However if δ is of the same order as ***machine precision***, then rounding errors could make ϵ somewhat larger than the above relation indicates. In fact ϵ will be largely independent of x or δ, but will be of the order of a few times the ***machine precision***.

8 Further Comments

None.

9 Example

The following program 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

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S15AFF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S15AFF
      EXTERNAL         S15AFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15AFF 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 = S15AFF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2 Program Data

```
S15AFF Example Program Data
            -2.0
            -0.5
             1.0
             1.5
             2.0
             5.0
            10.0
```

9.3 Program Results

```
 S15AFF Example Program Results

      X           Y        IFAIL

   -2.000E+00  -3.013E-01      0
   -5.000E-01  -4.244E-01      0
    1.000E+00   5.381E-01      0
    1.500E+00   4.282E-01      0
    2.000E+00   3.013E-01      0
    5.000E+00   1.021E-01      0
    1.000E+01   5.025E-02      0
```