NAG Library Routine Document

S15AFF

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 function name.

2 Specification

```
FUNCTION S15AFF (X, IFAIL)
REAL (KIND=nag_wp) S15AFF
INTEGER            IFAIL
REAL (KIND=nag_wp) X
```

3 Description

S15AFF 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 $0 < |x| \leq 4$,

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

For $|x| > 4$,

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

For $|x|$ near zero, $F(x) \simeq x$, and for $|x|$ large, $F(x) \simeq \dfrac{1}{2x}$. These approximations are used for those values of x for which the result is correct to ***machine precision***.

4 References

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

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 this routine.

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 $\left|\frac{x(1-2xF(x))}{F(x)}\right|$:

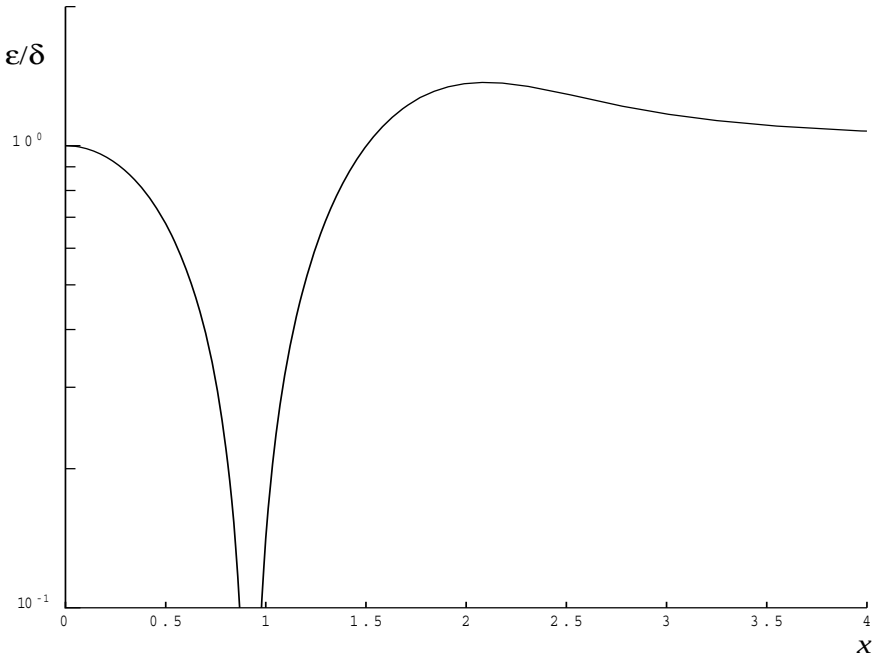

Figure 1

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 Parallelism and Performance

S15AFF 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 s15affe

!     S15AFF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, s15aff
!     .. 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,*) 'S15AFF 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 = s15aff(x,ifail)

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

99999 Format (1X,1P,2E12.3)
    End Program s15affe
```

10.2 Program Data

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

10.3 Program Results

```
 S15AFF Example Program Results

      X           Y

   -2.000E+00  -3.013E-01
   -5.000E-01  -4.244E-01
```

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