

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 routine name.

2 Specification

double precision FUNCTION S15AFF(X, IFAIL)
 INTEGER IFAIL
double precision 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 $0 < |x| \leq 4$,

$$F(x) = x \sum_{r=0}^l a_r T_r(t), \quad \text{where} \quad t = 2\left(\frac{x}{4}\right)^2 - 1.$$

For $|x| > 4$,

$$F(x) = \frac{1}{x} \sum_{r=0}^l b_r T_r(t), \quad \text{where} \quad t = 2\left(\frac{4}{x}\right)^2 - 1.$$

For $|x|$ near zero, $F(x) \simeq x$, and for $|x|$ large, $F(x) \simeq \frac{1}{2x}$. 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

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

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, if you are not familiar with this parameter, the recommended value is 0 . **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

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

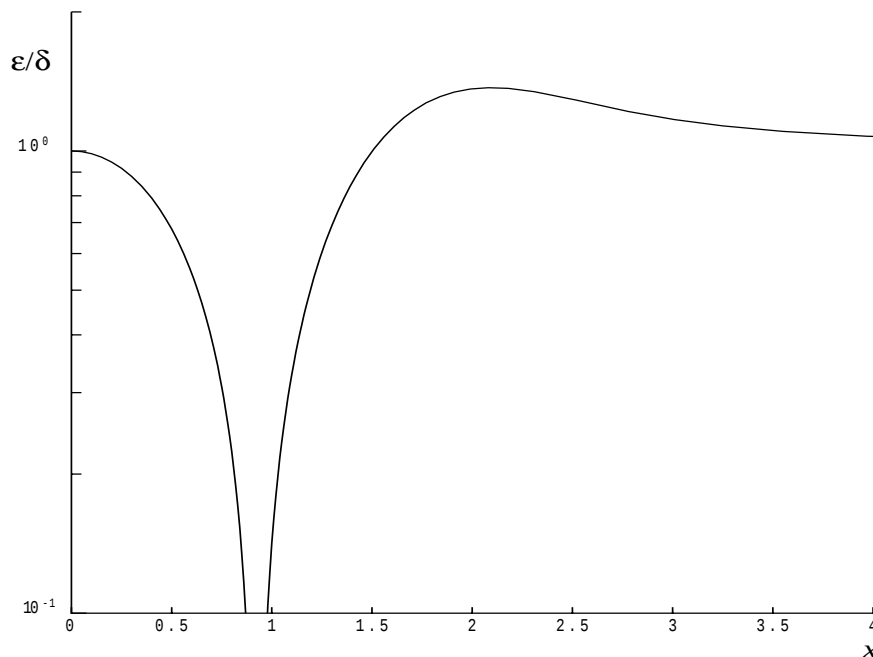


Figure 1

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 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

```

*      S15AFF Example Program Text
*      Mark 14 Revised. NAG Copyright 1989.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
      DOUBLE PRECISION X, Y
      INTEGER          IFAIL
*      .. External Functions ..
      DOUBLE PRECISION 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)
*
      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,2E12.3,I7)
99998  FORMAT (1X,' ** S15AFF returned with IFAIL = ',I5)
      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
