

NAG Fortran 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

```

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 $0 < |x| \leq 4$,

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

For $|x| > 4$,

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

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

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

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. Users who are unfamiliar with this parameter should refer to Chapter P01 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, for users 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 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 $\left| \frac{x(1 - 2xF(x))}{F(x)} \right|$:

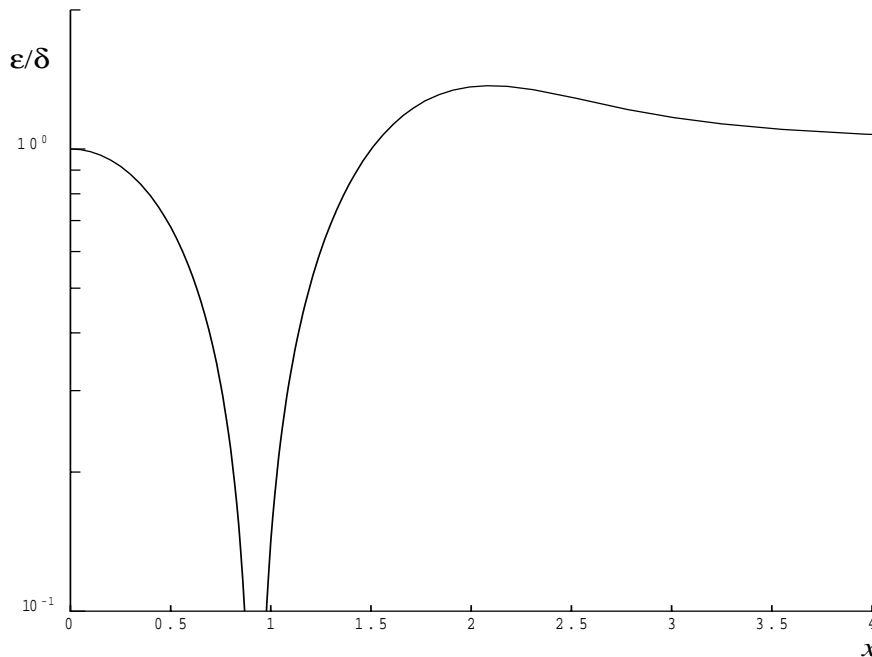


Figure 1

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 example 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
