NAG Library Routine Document

S13AAF

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.

Warning. The specification of the parameter X changed at Mark 21: X < 0.0 is no longer regarded as an input error.

1 Purpose

S13AAF returns the value of the exponential integral $E_1(x)$, via the routine name.

2 Specification

```
double precision FUNCTION S13AAF(X, IFAIL)
INTEGER                        IFAIL
double precision               X
```

3 Description

S13AAF calculates an approximate value for

$$E_1(x) = -\mathrm{Ei}(-x) = \int_x^\infty \frac{e^{-u}}{u} du.$$

using Chebyshev expansions, where x is real. For $x < 0$, the real part of the principal value of the integral is taken. The value $E_1(0)$ is infinite, and so, when $x = 0$, S13AAF exits with an error and returns the largest representable machine number.

For $0 < x \leq 4$,

$$E_1(x) = y(t) - \ln x = {\sum_r}' a_r T_r(t) - \ln x,$$

where $t = \frac{1}{2}x - 1$.

For $x > 4$,

$$E_1(x) = \frac{e^{-x}}{x} y(t) = \frac{e^{-x}}{x} {\sum_r}' a_r T_r(t),$$

where $t = -1.0 + \frac{14.5}{(x+3.25)} = \frac{11.25-x}{3.25+x}$.

In both cases, $-1 \leq t \leq +1$.

For $x < 0$, the approximation is based on expansions proposed by Cody and Thatcher Jr. (1969). Precautions are taken to maintain good relative accuracy in the vicinity of $x_0 \approx -0.372507\ldots$, which corresponds to a simple zero of $\mathrm{Ei}(-x)$.

S13AAF guards against producing underflows and overflows by using the parameter x_{hi}; see the Users' Note for your implementation for the value of x_{hi}. To guard against overflow, if $x < -x_{\mathrm{hi}}$ the routine terminates and returns the negative of the largest representable machine number. To guard against underflow, if $x > x_{\mathrm{hi}}$ the result is set directly to zero.

4 References

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

Cody WJ and Thatcher Jr. HC (1969) Rational Chebyshev approximations for the exponential integral $\mathrm{Ei}(x)$ *Math. Comp.* **23** 289–303

5 Parameters

1: X – ***double precision*** *Input*

On entry: the argument x of the function.

Constraint: $-x_{\mathrm{hi}} \leq \mathrm{X} < 0.0$ or $\mathrm{X} > 0.0$.

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: $\mathrm{IFAIL} = 0$ 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

If on entry $\mathrm{IFAIL} = 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

$\mathrm{IFAIL} = 1$

On entry, $\mathrm{X} = 0.0$ and the function is infinite. The result returned is the largest representable machine number.

$\mathrm{IFAIL} = 2$

The evaluation has been abandoned due to the likelihood of overflow. The argument $\mathrm{X} < -x_{\mathrm{hi}}$, and the result is returned as the negative of the largest representable machine number.

7 Accuracy

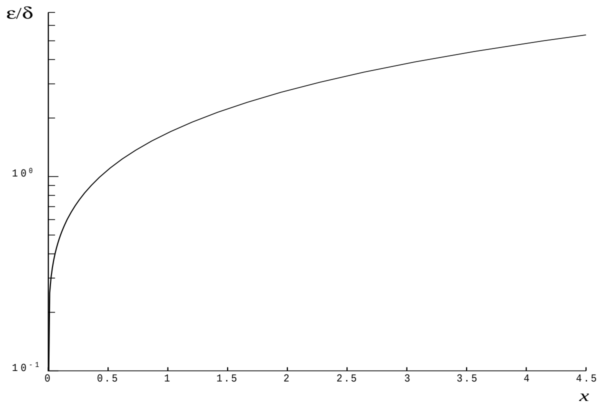
Unless stated otherwise, it is assumed that $x > 0$.

If δ and ϵ are the relative errors in argument and result respectively, then in principle,

$$|\epsilon| \simeq \left| \frac{e^{-x}}{E_1(x)} \times \delta \right|$$

so the relative error in the argument is amplified in the result by at least a factor $e^{-x}/E_1(x)$. The equality should hold if δ is greater than the ***machine precision*** (δ due to data errors etc.) but if δ is simply a result of round-off in the machine representation, it is possible that an extra figure may be lost in internal calculation and round-off.

The behaviour of this amplification factor is shown in the following graph:



It should be noted that, for absolutely small x, the amplification factor tends to zero and eventually the error in the result will be limited by ***machine precision***.

For absolutely large x,

$$\epsilon \sim x\delta = \Delta,$$

the absolute error in the argument.

For $x < 0$, empirical tests have shown that the maximum relative error is a loss of approximately 1 decimal place.

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

```
*     S13AAF 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 S13AAF
      EXTERNAL         S13AAF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S13AAF 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 = S13AAF(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,' ** S13AAF returned with IFAIL = ',I5)
      END
```

9.2 Program Data

```
S13AAF Example Program Data
             2.0
             0.0
            -1.0
         -1000.0
```

9.3 Program Results

```
 S13AAF Example Program Results

      X           Y        IFAIL

    2.000E+00   4.890E-02      0
    0.000E+00   1.798+308      1
   -1.000E+00  -1.895E+00      0
   -1.000E+03  -1.798+308      2
```