NAG Library Routine Document

S20AQF

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

S20AQF returns an array of values for the Fresnel integral $S(x)$.

2 Specification

```
SUBROUTINE S20AQF (N, X, F, IFAIL)

INTEGER              N, IFAIL
REAL (KIND=nag_wp) X(N), F(N)
```

3 Description

S20AQF evaluates an approximation to the Fresnel integral

$$S(x_i) = \int_0^{x_i} \sin\left(\frac{\pi}{2}t^2\right) dt$$

for an array of arguments x_i, for $i = 1, 2, \ldots, n$.

Note: $S(x) = -S(-x)$, so the approximation need only consider $x \geq 0.0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 3$,

$$S(x) = x^3 \sum_{r=0}{}' a_r T_r(t), \qquad \text{with } t = 2\left(\frac{x}{3}\right)^4 - 1.$$

For $x > 3$,

$$S(x) = \frac{1}{2} - \frac{f(x)}{x}\cos\left(\frac{\pi}{2}x^2\right) - \frac{g(x)}{x^3}\sin\left(\frac{\pi}{2}x^2\right),$$

where $f(x) = \sum_{r=0}{}' b_r T_r(t)$,

and $g(x) = \sum_{r=0}{}' c_r T_r(t)$,

with $t = 2\left(\frac{3}{x}\right)^4 - 1$.

For small x, $S(x) \simeq \frac{\pi}{6}x^3$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***. For very small x, this approximation would underflow; the result is then set exactly to zero.

For large x, $f(x) \simeq \frac{1}{\pi}$ and $g(x) \simeq \frac{1}{\pi^2}$. Therefore for moderately large x, when $\frac{1}{\pi^2 x^3}$ is negligible compared with $\frac{1}{2}$, the second term in the approximation for $x > 3$ may be dropped. For very large x, when $\frac{1}{\pi x}$ becomes negligible, $S(x) \simeq \frac{1}{2}$. However there will be considerable difficulties in calculating $\cos\left(\frac{\pi}{2}x^2\right)$ accurately before this final limiting value can be used. Since $\cos\left(\frac{\pi}{2}x^2\right)$ is periodic, its value is essentially determined by the fractional part of x^2. If $x^2 = N + \theta$ where N is an integer and $0 \leq \theta < 1$, then $\cos\left(\frac{\pi}{2}x^2\right)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain significance in the calculation of $\cos\left(\frac{\pi}{2}x^2\right)$ either all the way to the very large x limit, or at least until the integer part of $\frac{x}{2}$ is equal to the maximum integer allowed on the machine.

4 References

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

5 Parameters

1: N – INTEGER *Input*

On entry: n, the number of points.

Constraint: $\mathrm{N} \geq 0$.

2: X(N) – REAL (KIND=nag_wp) array *Input*

On entry: the argument x_i of the function, for $i = 1, 2, \ldots, \mathrm{N}$.

3: F(N) – REAL (KIND=nag_wp) array *Output*

On exit: $S(x_i)$, the function values.

4: 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.

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.**

On exit: $\mathrm{IFAIL} = 0$ unless the routine detects an error or a warning has been flagged (see Section 6).

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, $\mathrm{N} = \langle value \rangle$.
Constraint: $\mathrm{N} \geq 0$.

7 Accuracy

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

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

$$\epsilon \simeq \left| \frac{x \sin\left(\frac{\pi}{2}x^2\right)}{S(x)} \right| \delta.$$

Figure 1 shows the behaviour of the error amplification factor $\left|\dfrac{x\sin\left(\frac{\pi}{2}x^2\right)}{S(x)}\right|$.

However if δ is of the same order as the ***machine precision***, then rounding errors could make ϵ slightly larger than the above relation predicts.

For small x, $\epsilon \simeq 3\delta$ and hence there is only moderate amplification of relative error. Of course for very small x where the correct result would underflow and exact zero is returned, relative error-control is lost.

For moderately large values of x,

$$\epsilon \simeq \left|2x\sin\left(\frac{\pi}{2}x^2\right)\right|\delta$$

and the result will be subject to increasingly large amplification of errors. However the above relation breaks down for large values of x (i.e., when $\dfrac{1}{x^2}$ is of the order of the ***machine precision***); in this region the relative error in the result is essentially bounded by $\dfrac{2}{\pi x}$.

Hence the effects of error amplification are limited and at worst the relative error loss should not exceed half the possible number of significant figures.

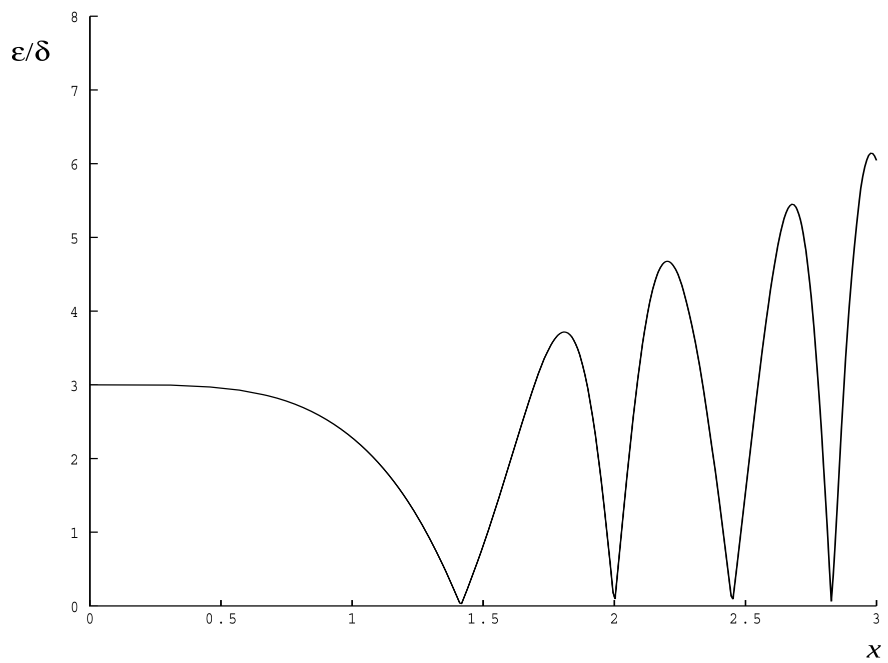

Figure 1

8 Further Comments

None.

9 Example

This example reads values of X from a file, evaluates the function at each value of x_i and prints the results.

9.1 Program Text

```
    Program s20aqfe

!     S20AQF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, s20aqf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nin = 5, nout = 6
!     .. Local Scalars ..
      Integer                          :: i, ifail, n
!     .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable  :: f(:), x(:)
!     .. Executable Statements ..
      Write (nout,*) 'S20AQF Example Program Results'

!     Skip heading in data file
      Read (nin,*)

      Write (nout,*)
      Write (nout,*) '     X           F'
      Write (nout,*)

      Read (nin,*) n

      Allocate (x(n),f(n))

      Read (nin,*) x(1:n)

      ifail = 0
      Call s20aqf(n,x,f,ifail)

      Do i = 1, n
        Write (nout,99999) x(i), f(i)
      End Do

99999 Format (1X,1P,2E12.3)
    End Program s20aqfe
```

9.2 Program Data

```
S20AQF Example Program Data

11

0.0 0.5 1.0 2.0 4.0 5.0 6.0 8.0 10.0 -1.0 1000.0
```

9.3 Program Results

```
 S20AQF Example Program Results

      X           F

    0.000E+00   0.000E+00
    5.000E-01   6.473E-02
    1.000E+00   4.383E-01
    2.000E+00   3.434E-01
    4.000E+00   4.205E-01
    5.000E+00   4.992E-01
    6.000E+00   4.470E-01
    8.000E+00   4.602E-01
    1.000E+01   4.682E-01
   -1.000E+00  -4.383E-01
    1.000E+03   4.997E-01
```