NAG Toolbox

nag_specfun_fresnel_s_vector (s20aq)

1 Purpose

nag_specfun_fresnel_s_vector (s20aq) returns an array of values for the Fresnel integral $S(x)$.

2 Syntax

```
[f, ifail] = nag_specfun_fresnel_s_vector(x, 'n', n)
[f, ifail] = s20aq(x, 'n', n)
```

3 Description

nag_specfun_fresnel_s_vector (s20aq) 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 function 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

5.1 Compulsory Input Parameters

1: **x**(**n**) – REAL (KIND=nag_wp) array

The argument x_i of the function, for $i = 1, 2, \ldots, \mathbf{n}$.

5.2 Optional Input Parameters

1: **n** – INTEGER

Default: the dimension of the array **x**.

n, the number of points.

Constraint: $\mathbf{n} \geq 0$.

5.3 Output Parameters

1: **f**(**n**) – REAL (KIND=nag_wp) array

$S(x_i)$, the function values.

2: **ifail** – INTEGER

ifail $= 0$ unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= 1$ (*warning*)

Constraint: $\mathbf{n} \geq 0$.

ifail $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

ifail $= -399$

Your licence key may have expired or may not have been installed correctly.

ifail $= -999$

Dynamic memory allocation failed.

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

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 $\frac{1}{x^2}$ is of the order of the ***machine precision***); in this region the relative error in the result is essentially bounded by $\frac{2}{\pi x}$.

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.

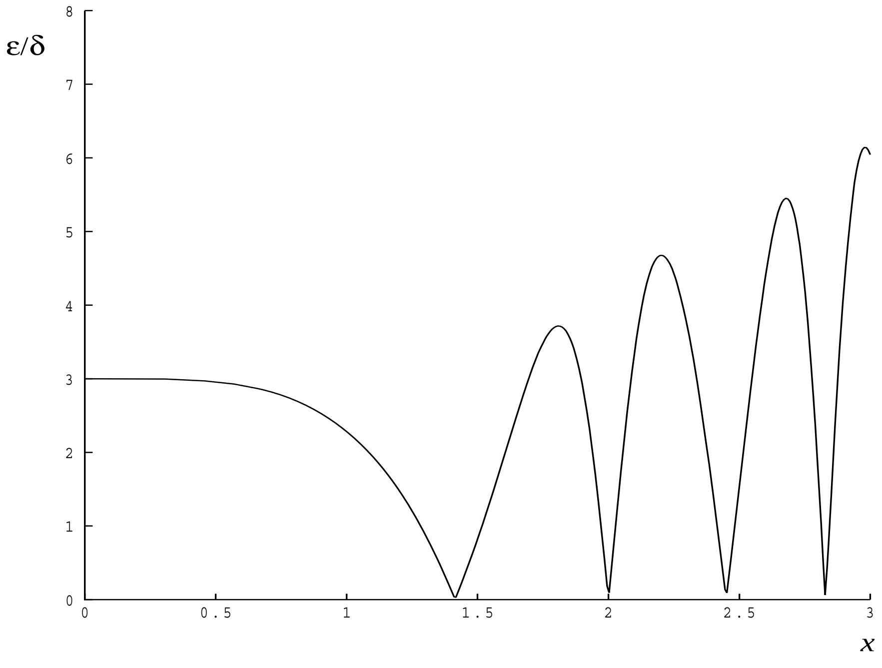

Figure 1

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

```
     function s20aq_example

fprintf('s20aq example results\n\n');

x = [0; 0.5; 1; 2; 4; 5; 6; 8; 10; -1; 1000];

[f, ifail] = s20aq(x);

fprintf('     x           S(x)\n');
for i=1:numel(x)
  fprintf('%12.3e%12.3e\n', x(i), f(i));
end
```

9.2 Program Results

```
     s20aq example results

     x           S(x)
   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
```