NAG Library Function Document

nag_fresnel_s_vector (s20aqc)

1 Purpose

nag_fresnel_s_vector (s20aqc) returns an array of values for the Fresnel integral $S(x)$.

2 Specification

```
#include <nag.h>
#include <nags.h>
void nag_fresnel_s_vector (Integer n, const double x[], double f[],
     NagError *fail)
```

3 Description

nag_fresnel_s_vector (s20aqc) 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 Arguments

1: **n** – Integer *Input*

On entry: n, the number of points.

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

2: **x**[**n**] – const double *Input*

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

3: **f**[**n**] – double *Output*

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

4: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument ⟨*value*⟩ had an illegal value.

NE_INT

On entry, $\mathbf{n} = \langle value \rangle$.
Constraint: $\mathbf{n} \geq 0$.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

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.

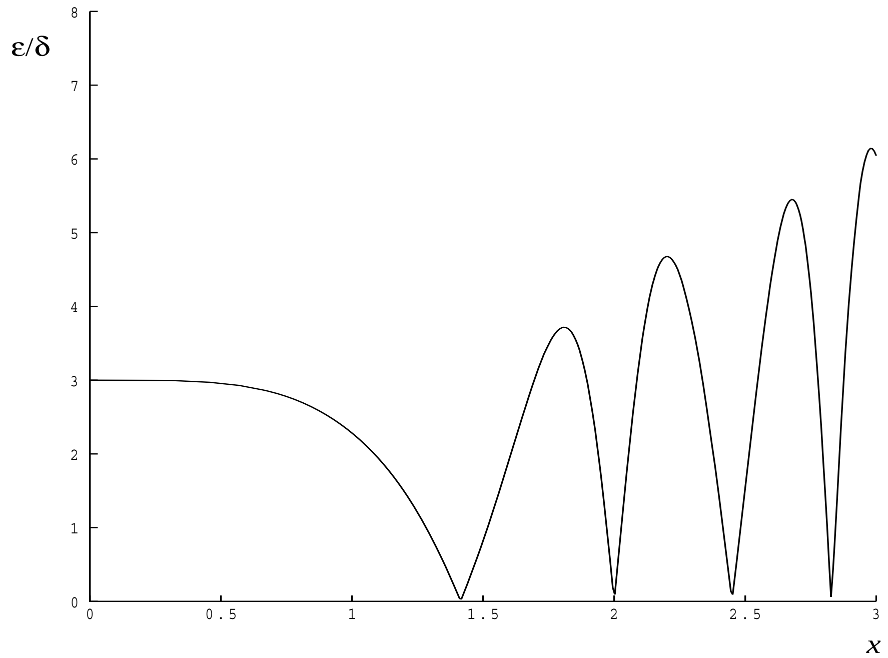

Figure 1

8 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 Example

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

10.1 Program Text

```
/* nag_fresnel_s_vector (s20aqc) Example Program.
 *
 * Copyright 2011, Numerical Algorithms Group.
 *
 * Mark 23 2011.
 */
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nags.h>

int main(void)
{
  Integer  exit_status = 0;
  Integer  i, n;
  double   *f = 0, *x = 0;
  NagError fail;

  INIT_FAIL(fail);

  /* Skip heading in data file */
  scanf("%*[^\n]");

  printf("nag_fresnel_s_vector (s20aqc) Example Program Results\n");
  printf("\n");
  printf("     x           f\n");
  printf("\n");
  scanf("%ld", &n);
  scanf("%*[^\n]");

  /* Allocate memory */
  if (!(x = NAG_ALLOC(n, double)) ||
      !(f = NAG_ALLOC(n, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  for (i=0; i<n; i++)
    scanf("%lf", &x[i]);
  scanf("%*[^\n]");

  /* nag_fresnel_s_vector (s20aqc).
   * Fresnel Integral S(x)
   */
  nag_fresnel_s_vector(n, x, f, &fail);
  if (fail.code!=NE_NOERROR)
    {
      printf("Error from nag_fresnel_s_vector (s20aqc).\n%s\n",
             fail.message);
      exit_status = 1;
      goto END;
    }

  for (i=0; i<n; i++)
    printf(" %11.3e %11.3e\n", x[i], f[i]);

 END:
  NAG_FREE(f);
  NAG_FREE(x);

  return exit_status;
}
```

10.2 Program Data

```
nag_fresnel_s_vector (s20aqc) Example Program Data

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

10.3 Program Results

```
nag_fresnel_s_vector (s20aqc) 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
```