Module 3.5: nag_fresnel_intg

Fresnel Integrals

`nag_fresnel_intg` contains procedures for approximating the Fresnel integrals $S(x)$ and $C(x)$.

Contents

Introduction

This module contains procedures for approximating Fresnel integrals.

- `nag_fresnel_s` approximates the Fresnel integral

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

- `nag_fresnel_c` approximates the Fresnel integral

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right) dt.$$

Further details of Fresnel integrals may be found in Abramowitz and Stegun [1], Chapter 7.

In general the approximations are based on expansions in terms of Chebyshev polynomials $T_r(t) = \cos(r \arccos t)$. Further details appear in Section 6.1 of the individual procedure documents.

Procedure: nag_fresnel_s

1 Description

nag_fresnel_s evaluates an approximation to the Fresnel integral

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

2 Usage

```
USE nag_fresnel_intg
[value =] nag_fresnel_s(x)
```

The function result is a scalar, of type real(kind=*wp*), containing $S(x)$.

3 Arguments

3.1 Mandatory Argument

x — real(kind=*wp*), intent(in)
Input: the argument x of the function.

4 Error Codes

None.

5 Examples of Usage

A complete example of the use of this procedure appears in Example 1 of this module document.

6 Further Comments

6.1 Algorithmic Detail

Since $S(x) = -S(-x)$ it is only necessary to consider the case $x \geq 0.0$.

- For $0 < x \leq 3$, the procedure uses a Chebyshev expansion of the form

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

- For $x > 3$, it uses

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

  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, $S(x) \simeq \pi x^3/6$. This approximation is used when x is sufficiently small for the result to be correct to EPSILON(1.0_*wp*). For very small x, this approximation would underflow; the result is then set exactly to zero.

- For large x, $f(x) \simeq 1/\pi$ and $g(x) \simeq 1/\pi^2$. Therefore for moderately large x, when $1/(\pi^2 x^3)$ is negligible compared with 0.5, the second term in the approximation for $x > 3$ may be dropped. For very large x, when $1/(\pi x)$ becomes negligible, $S(x) \simeq 0.5$. However there will be considerable difficulties in calculating $\cos(\pi x^2/2)$ accurately before this final limiting value can be used. Since $\cos(\pi x^2/2)$ 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 $0 \le \theta < 1$, then $\cos(\pi x^2/2)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain significance in the calculation of $\cos(\pi x^2/2)$ either all the way to the very large x limit or at least until the integer part of $x/2$ is equal to the maximum integer allowed on the machine.

6.2 Accuracy

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

If δ is somewhat larger than EPSILON(1.0_*wp*) (i.e., if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq |\theta|\delta, \quad \text{where} \quad \theta = \frac{x\sin(\pi x^2/2)}{S(x)}.$$

The behaviour of the error amplification factor $|\theta|$ is shown in Figure 1.

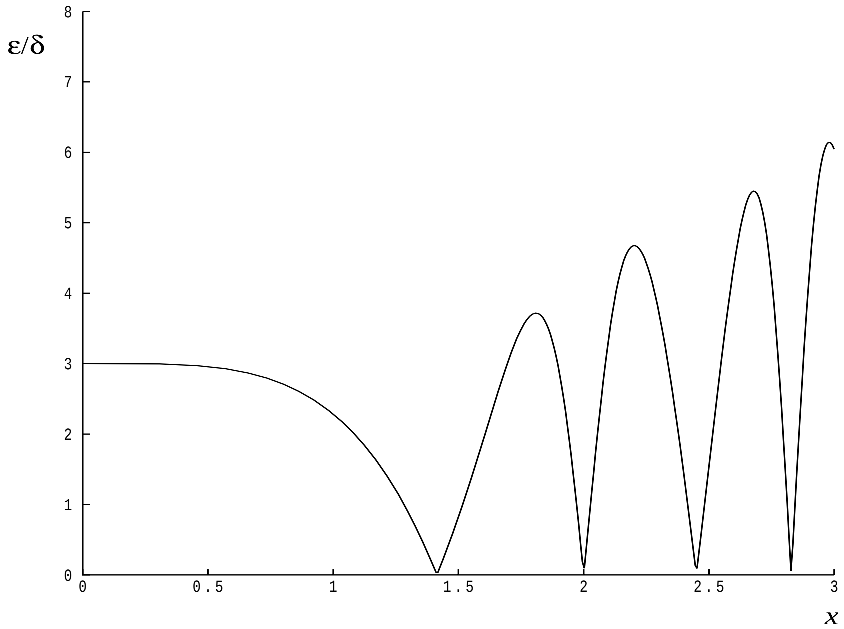

Figure 1: The error amplification factor $|\theta|$.

However, if δ is of the same order as EPSILON(1.0_*wp*), then rounding errors could make ε slightly larger than the above relation predicts.

For small x, $\varepsilon \simeq 3\delta$ 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, $|\varepsilon| \simeq |2x\sin(\pi x^2/2)||\delta|$ 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 $1/x^2$ is of the order of EPSILON(1.0_*wp*); in this region the relative error in the result is essentially bounded by $2/(\pi x)$).

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.

Procedure: nag_fresnel_c

1 Description

nag_fresnel_c evaluates an approximation to the Fresnel integral

$$C(x) = \int_0^x \cos\left(\pi t^2/2\right) dt.$$

2 Usage

```
USE nag_fresnel_intg
[value =] nag_fresnel_c(x)
```

The function result is a scalar, of type real(kind=*wp*), containing $C(x)$.

3 Arguments

3.1 Mandatory Argument

x — real(kind=*wp*), intent(in)
Input: the argument x of the function.

4 Error Codes

None.

5 Examples of Usage

A complete example of the use of this procedure appears in Example 1 of this module document.

6 Further Comments

6.1 Algorithmic Detail

Since $C(x) = -C(-x)$ it is only necessary to consider the case $x \geq 0.0$.

- For $0 < x \leq 3$, the procedure uses a Chebyshev expansion of the form

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

- For $x > 3$, it uses

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

  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, $C(x) \simeq x$. This approximation is used when x is sufficiently small for the result to be correct to EPSILON(1.0_*wp*).

- For large x, $f(x) \simeq 1/\pi$ and $g(x) \simeq 1/\pi^2$. Therefore for moderately large x, when $1/(\pi^2 x^3)$ is negligible compared with 0.5, the second term in the approximation for $x > 3$ may be dropped. For very large x, when $1/(\pi x)$ becomes negligible, $C(x) \simeq 0.5$. However there will be considerable difficulties in calculating $\sin(\pi x^2/2)$ accurately before this final limiting value can be used. Since $\sin(\pi x^2/2)$ 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 $\sin(\pi x^2/2)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain some significance in the calculation of $\sin(\pi x^2/2)$ either all the way to the very large x limit or at least until the integer part of $x/2$ is equal to the maximum integer allowed on the machine.

6.2 Accuracy

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

If δ is somewhat larger than EPSILON(1.0_*wp*) (i.e., if δ is due to data errors etc.), then ε and δ are approximately related by:

$$\varepsilon \simeq |\theta|\delta, \quad \text{where} \quad \theta = \frac{x\cos(\pi x^2/2)}{C(x)}.$$

The behaviour of the error amplification factor $|\theta|$ is shown in Figure 2.

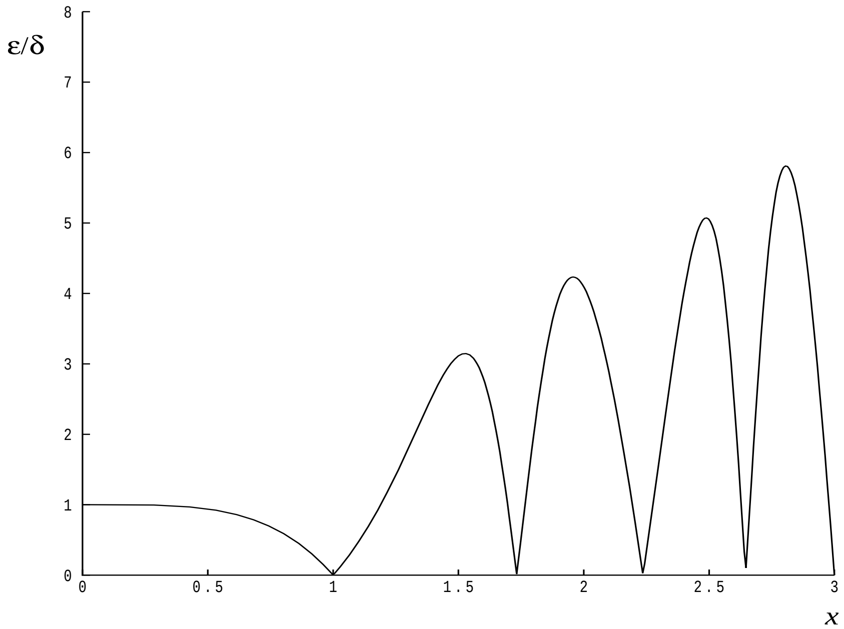

Figure 2: The error amplification factor $|\theta|$.

However if δ is of the same order as EPSILON(1.0_*wp*), then rounding errors could make ε slightly larger than the above relation predicts.

For small x, $\varepsilon \simeq \delta$ and there is no amplification of relative error.

For moderately large values of x, $|\varepsilon| \simeq |2x\cos(\pi x^2/2)||\delta|$ 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 $1/x^2$ is of the order of EPSILON(1.0_*wp*)); in this region the relative error in the result is essentially bounded by $2/(\pi x)$).

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.

Example 1: Evaluation of the Fresnel Integrals

This example program evaluates the functions `nag_fresnel_s` and `nag_fresnel_c` at a set of values of the argument `x`.

1 Program Text

Note. The listing of the example program presented below is double precision. Single precision users are referred to Section 5.2 of the Essential Introduction for further information.

```
PROGRAM nag_fresnel_intg_ex01

  ! Example Program Text for nag_fresnel_intg
  ! NAG fl90, Release 3. NAG Copyright 1997.

  ! .. Use Statements ..
  USE nag_examples_io, ONLY : nag_std_out
  USE nag_fresnel_intg, ONLY : nag_fresnel_s, nag_fresnel_c
  ! .. Implicit None Statement ..
  IMPLICIT NONE
  ! .. Intrinsic Functions ..
  INTRINSIC KIND
  ! .. Parameters ..
  INTEGER, PARAMETER :: n = 11
  INTEGER, PARAMETER :: wp = KIND(1.0D0)
  ! .. Local Scalars ..
  INTEGER :: i
  REAL (wp) :: c_x, s_x
  ! .. Local Arrays ..
  REAL (wp) :: x(n)
  ! .. Executable Statements ..

  WRITE (nag_std_out,*) &
   'Example Program Results for nag_fresnel_intg_ex01'

  WRITE (nag_std_out,*)
  WRITE (nag_std_out,*) '      x          S(x)        C(x)'
  x = (/ -1.0_wp, 0.0_wp, 0.5_wp, 1.0_wp, 2.0_wp, 4.0_wp, 5.0_wp, 6.0_wp, &
   8.0_wp, 10.0_wp, 1000.0_wp/)

  DO i = 1, n

    s_x = nag_fresnel_s(x(i))
    c_x = nag_fresnel_c(x(i))

    WRITE (nag_std_out,fmt='(1X,1P,3E12.3)') x(i), s_x, c_x
  END DO

END PROGRAM nag_fresnel_intg_ex01
```

2 Program Data

None.

3 Program Results

```
 Example Program Results for nag_fresnel_intg_ex01

       x          S(x)        C(x)
   -1.000E+00  -4.383E-01  -7.799E-01
    0.000E+00   0.000E+00   0.000E+00
    5.000E-01   6.473E-02   4.923E-01
    1.000E+00   4.383E-01   7.799E-01
    2.000E+00   3.434E-01   4.883E-01
    4.000E+00   4.205E-01   4.984E-01
    5.000E+00   4.992E-01   5.636E-01
    6.000E+00   4.470E-01   4.995E-01
    8.000E+00   4.602E-01   4.998E-01
    1.000E+01   4.682E-01   4.999E-01
    1.000E+03   4.997E-01   5.000E-01
```

Additional Examples

Not all example programs supplied with NAG *fl*90 appear in full in this module document. The following additional examples, associated with this module, are available.

`nag_fresnel_intg_ex02`

Evaluation of the Fresnel integral $S(x)$.

`nag_fresnel_intg_ex03`

Evaluation of the Fresnel integral $C(x)$.

References

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