NAG Library Function Document

nag_erfcx (s15agc)

1 Purpose

nag_erfcx (s15agc) returns the value of the scaled complementary error function erfcx(x).

2 Specification

```
#include <nag.h>
#include <nags.h>
double nag_erfcx (double x, NagError *fail)
```

3 Description

nag_erfcx (s15agc) calculates an approximate value for the scaled complementary error function

$$\text{erfcx}(x) = e^{x^2}\,\text{erfc}(x) = \frac{2}{\sqrt{\pi}}e^{x^2}\int_x^\infty e^{-t^2}\,dt = e^{x^2}(1-\text{erf}(x)).$$

Let $\hat{x}$ be the root of the equation $\text{erfc}(x) - \text{erf}(x) = 0$ (then $\hat{x} \approx 0.46875$). For $|x| \leq \hat{x}$ the value of erfcx(x) is based on the following rational Chebyshev expansion for erf(x):

$$\text{erf}(x) \approx xR_{\ell,m}\left(x^2\right),$$

where $R_{\ell,m}$ denotes a rational function of degree ℓ in the numerator and m in the denominator.

For $|x| > \hat{x}$ the value of erfcx(x) is based on a rational Chebyshev expansion for erfc(x): for $\hat{x} < |x| \leq 4$ the value is based on the expansion

$$\text{erfc}(x) \approx e^{x^2}R_{\ell,m}(x);$$

and for $|x| > 4$ it is based on the expansion

$$\text{erfc}(x) \approx \frac{e^{x^2}}{x}\left(\frac{1}{\sqrt{\pi}} + \frac{1}{x^2}R_{\ell,m}\left(1/x^2\right)\right).$$

For each expansion, the specific values of ℓ and m are selected to be minimal such that the maximum relative error in the expansion is of the order 10^{-d}, where d is the maximum number of decimal digits that can be accurately represented for the particular implementation (see nag_decimal_digits (X02BEC)).

Asymptotically, erfcx$(x) \sim 1/(\sqrt{\pi}|x|)$. There is a danger of setting underflow in erfcx(x) whenever $x \geq x_{\text{hi}} = \min\left(x_{\text{huge}}, 1/\left(\sqrt{\pi}x_{\text{tiny}}\right)\right)$, where x_{huge} is the largest positive model number (see nag_real_largest_number (X02ALC)) and x_{tiny} is the smallest positive model number (see nag_real_smallest_number (X02AKC)). In this case nag_erfcx (s15agc) exits with **fail**.**code** = NW_HI and returns erfcx$(x) = 0$. For x in the range $1/(2\sqrt{\epsilon}) \leq x < x_{\text{hi}}$, where ϵ is the ***machine precision***, the asymptotic value $1/(\sqrt{\pi}|x|)$ is returned for erfcx(x) and nag_erfcx (s15agc) exits with **fail**.**code** = NW_REAL.

There is a danger of setting overflow in e^{x^2} whenever $x < x_{\text{neg}} = -\sqrt{\log\left(x_{\text{huge}}/2\right)}$. In this case nag_erfcx (s15agc) exits with **fail**.**code** = NW_NEG and returns erfcx$(x) = x_{\text{huge}}$.

The values of x_{hi}, $1/(2\sqrt{\epsilon})$ and x_{neg} are given in the Users' Note for your implementation.

4 References

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

Cody W J (1969) Rational Chebyshev approximations for the error function *Math.Comp.* **23** 631–637

5 Arguments

1: **x** – double *Input*

On entry: the argument x of the function.

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

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

6 Error Indicators and Warnings

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.

NW_HI

On entry, $\mathbf{x} = \langle value \rangle$ and the constant $x_{\mathrm{hi}} = \langle value \rangle$.
Constraint: $\mathbf{x} < x_{\mathrm{hi}}$.

NW_NEG

On entry, $\mathbf{x} = \langle value \rangle$ and the constant $x_{\mathrm{neg}} = \langle value \rangle$.
Constraint: $\mathbf{x} \geq x_{\mathrm{neg}}$.

NW_REAL

On entry, $|\mathbf{x}|$ was in the interval $[\langle value \rangle, \langle value \rangle)$ where erfcx($\mathbf{x}$) is approximately $1/(\sqrt{\pi} * |\mathbf{x}|)$: $\mathbf{x} = \langle value \rangle$.

7 Accuracy

The relative error in computing erfcx(x) may be estimated by evaluating

$$E = \frac{\mathrm{erfcx}(x) - e^{x^2} \sum_{n=1}^{\infty} I^n \,\mathrm{erfc}(x)}{\mathrm{erfcx}(x)},$$

where I^n denotes repeated integration. Empirical results suggest that on the interval $(\hat{x}, 2)$ the loss in base b significant digits for maximum relative error is around 3.3, while for root-mean-square relative error on that interval it is 1.2 (see nag_real_base (X02BHC) for the definition of the model parameter b). On the interval $(2, 20)$ the values are around 3.5 for maximum and 0.45 for root-mean-square relative errors; note that on these two intervals erfc(x) is the primary computation. See also Section 7 in nag_erfc (s15adc).

8 Parallelism and Performance

Not applicable.

9 Further Comments

None.

10 Example

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

10.1 Program Text

```
/* nag_erfcx (s15agc) Example Program.
 *
 * Copyright 2008, Numerical Algorithms Group.
 *
 * Mark 9, 2009.
 */
/* Pre-processor includes */
#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nags.h>
int main(void)
{
  /*Integer scalar and array declarations */
  Integer    exit_status = 0;
  /*Double scalar and array declarations */
  double     x, y;

  NagError   fail;
  const char *str_fail;

  INIT_FAIL(fail);

  printf("nag_erfcx (s15agc) Example Program Results\n");
  /* Skip heading in data file*/
  scanf("%*[^\n] ");
  printf("\n%s\n\n", "       x          erfcx(x)     fail");
  while (scanf("%lf%*[^\n] ", &x) != EOF)
    {
      /*
       * nag_erfcx (s15agc)
       * Scaled complement of error function, erfcx(x)
       */
      y = nag_erfcx(x, &fail);
      if (fail.code != NE_NOERROR)
        {
          if (fail.code == NW_HI || fail.code == NW_NEG ||
              fail.code == NW_REAL)
            {
              /* nag_code_to_error_name (x04ndc).
               * Converts NAG error code to its string value
               */
              str_fail = nag_code_to_error_name(fail.code);
              printf("%14.5e  %-14.5e %s\n", x, y, str_fail);
            }
          else
            {
              printf("Error from nag_erfcx (s15agc).\n%s\n",
                      fail.message);
              exit_status = 1;
              goto END;
            }
        }
      else
        {
          printf("%14.5e  %-14.5e\n", x, y);
        }
```

```
    }

 END:

  return exit_status;
}
```

10.2 Program Data

```
nag_erfcx (s15agc) Example Program Data
            -30.0
            -6.0
            -4.5
            -1.0
             1.0
             4.5
             6.0
             70000000.0
```

10.3 Program Results

```
nag_erfcx (s15agc) Example Program Results

       x          erfcx(x)     fail

 -3.00000e+01  1.79769e+308    NW_NEG
 -6.00000e+00  8.62246e+15
 -4.50000e+00  1.24593e+09
 -1.00000e+00  5.00898e+00
  1.00000e+00  4.27584e-01
  4.50000e+00  1.22485e-01
  6.00000e+00  9.27766e-02
  7.00000e+07  8.05985e-09     NW_REAL
```