NAG Toolbox for Matlab

s15ag

1 Purpose
s15ag returns the value of the scaled complementary error function $\text{erfcx}(x)$, via the function name.

2 Syntax

$$[\text{result, } \text{ifail}] = \text{s15ag}(x)$$

3 Description
s15ag calculates an approximate value for the scaled complementary error function

$$\text{erfcx}(x) = e^{-x^2} \text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt = e^{-x^2} (1 - \text{erf}(x)).$$

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 $\text{erfcx}(x)$ is based on the following rational Chebyshev expansion for $\text{erf}(x)$:

$$\text{erf}(x) \approx x R_{\ell,m}(x^2),$$

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

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

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

For each expansion, the specific values of $\ell$ 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 x02be).

Asymptotically, $\text{erfcx}(x) \sim 1/(\sqrt{\pi} \text{abs}(x))$. There is a danger of setting underflow in $\text{erfcx}(x)$ whenever $x \geq x_{\text{hi}} = \min(x_{\text{huge}}, 1/(\sqrt{\pi} x_{\text{tiny}}))$, where $x_{\text{huge}}$ is the largest positive model number (see x02al) and $x_{\text{tiny}}$ is the smallest positive model number (see x02ak). In this case s15ag exits with $\text{ifail} = 1$ and returns $\text{erfcx}(x) = 0$. For $x$ in the range $1/(2\sqrt{\epsilon}) \leq x < x_{\text{hi}}$, where $\epsilon$ is the machine precision, the asymptotic value $1/(\sqrt{\pi} \text{abs}(x))$ is returned for $\text{erfcx}(x)$ and s15ag exits with $\text{ifail} = 2$.

There is a danger of setting overflow in $e^{-x^2}$ whenever $x < x_{\text{neg}} = -\sqrt{\log(x_{\text{huge}}/2)}$. In this case s15ag exits with $\text{ifail} = 3$ and returns $\text{erfcx}(x) = x_{\text{huge}}$.

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

4 References
5 Parameters

5.1 Compulsory Input Parameters

1: \( x \) – double scalar
   The argument \( x \) of the function.

5.2 Optional Input Parameters

None.

5.3 Input Parameters Omitted from the MATLAB Interface

None.

5.4 Output Parameters

1: \( \text{result} \) – double scalar
   The result of the function.

2: \( \text{ifail} \) – int32 scalar
   \( \text{ifail} = 0 \) unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Note: s15ag may return useful information for one or more of the following detected errors or warnings.

Errors or warnings detected by the function:

\( \text{ifail} = 1 \)

On entry, \( x \geq x_{\text{hi}} \) (see Section 3). On soft failure the function value returned is 0.

\( \text{ifail} = 2 \)

On entry, \( 1/(2\sqrt{e}) \leq x < x_{\text{hi}} \) (see Section 3). On soft failure the function value returned is \( 1/(\sqrt{\pi} \text{abs}(x)) \).

\( \text{ifail} = 3 \)

On entry, \( x < x_{\text{neg}} \) (see Section 3). On soft failure the function value returned is the largest positive model number.

7 Accuracy

The relative error in computing \( \text{erfcx}(x) \) may be estimated by evaluating

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

where \( I^n \) denotes repeated integration. Empirical results suggest that on the interval \((x, 2)\) 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 x02bh for the definition of the model parameter \( b \)). On the interval \((2, 20)\) the values are around 2.0 for maximum and 0.05 for root-mean-square relative errors; note that on these two intervals \( \text{erfc}(x) \) is the primary computation. See also Section 7 in s15ad.
8 Further Comments

None.

9 Example

```matlab
x = [-30.0; -6.0; -4.5; -1.0; 1.0; 4.5; 6.0; 7.0e7];
result = zeros(8, 1);
ifail = zeros(8, 1, 'int32');
for i=1:8
    [result(i), ifail(i)] = s15ag(x(i));
end
fprintf(' x erfcx(x) ifail
');
for i=1:8
    fprintf('%13.5e %13.5e %d
', x(i), result(i), ifail(i));
end
% The first number returned is too big to be input into Matlab
% Compare the logs to avoid differences in least significant digit
```

Warning: s15ag returned a non-zero warning or error indicator (3)

Warning: s15ag returned a non-zero warning or error indicator (2)

```matlab
x erfcx(x) ifail
-3.00000e+01  1.79769e+308  3
-6.00000e+00  8.62246e+15   0
-4.50000e+00  1.24593e+09   0
-1.00000e+00  5.00898e+00   0
 1.00000e+00  4.27584e-01   0
 4.50000e+00  1.22485e-01   0
 6.00000e+00  9.27766e-02   0
 7.00000e+07  8.05985e-09   2
```