2.2 Error Function, Gaussian Probability Integral, etc.

A. Purpose

These subprograms compute values of the error function, the complementary error function, and an exponentially scaled complementary error function, [1, 2]. The closely related Gaussian or normal probability integral can be computed by subprograms described in Chapter 15.2.

Error function:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$

Complementary error function:

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

Exponentially scaled complementary error function:

$$\mathrm{erfce}(x) = \exp(x^2)\ \mathrm{erfc}(x)$$

B. Usage

B.1 Program Prototype, Single Precision

REAL X, Y, SERF, SERFC, SERFCE

Assign a value to X and obtain the value of erf, erfc, or erfce, respectively, as follows:

Y = SERF(X)   **Y = SERFC(X)**

Y = SERFCE(X)

B.2 Argument Definitions

X [in] Argument at which function evaluation is desired. Require X ≥ 0 when using SERFCE.

Y [out] Value of function returned.

B.3 Modifications for Double Precision

For double precision change the REAL type statement to DOUBLE PRECISION and change the function names to DERF, DERFC, and DERFCE.

C. Examples and Remarks

See DRSERF and ODSERF for an example of the usage of these subprograms.

The ANSI Fortran 77 standard does not include the error function, or the related functions, erfc and erfce, as intrinsic functions. Some Fortran systems, however, do provide such functions. For example, UNISYS ASCII Fortran and IBM VS-Fortran provide ERF, ERFC, DERF, and DERFC, with ERF and ERFC being "generic," whereas VAX-11 Fortran does not provide these functions.

In a system having DERF or DERFC as intrinsics, a reference to one of these function names will cause the vendor-supplied code to be used. If one wishes to override this and use the code from this library one must declare the function name to be EXTERNAL in the referencing program unit.

Whenever the user's mathematical problem involves the expression, $1 - \mathrm{erf}(x)$, $\mathrm{erfc}(x)$ should be used instead. This will give significantly better relative accuracy as x increases above 0.5, and no worse accuracy for $x < 0.5$.

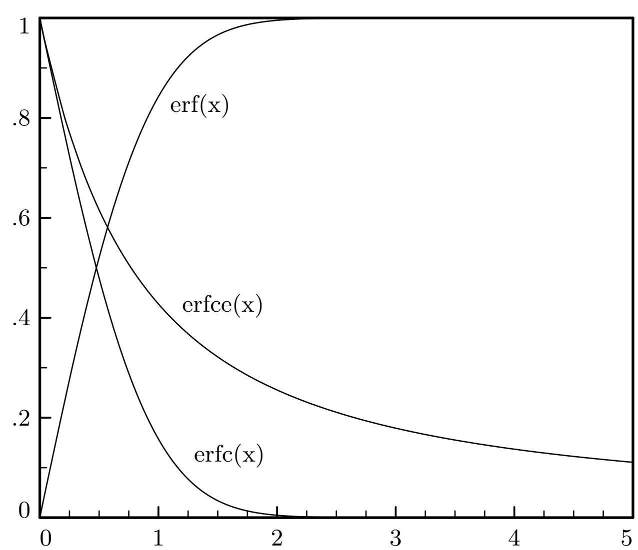
In cases in which the user's problem involves the expression, $\exp(x^2)[1 - \mathrm{erf}(x)]$, with $x \geq 0$, $\mathrm{erfce}(x)$ should be used. This avoids the problem of $\exp(x^2)$ reaching the overflow limit for fairly modest values of x, since $\mathrm{erfce}(x)$ is asymptotic to $1/(x\ \pi^{1/2})$ as x approaches infinity.

D. Functional Description

The function $\mathrm{erf}(x)$ is an odd function, increasing monotonically from -1 at $x = -\infty$ to $+1$ at $x = +\infty$. The function $\mathrm{erfc}(x) = 1 - \mathrm{erf}(x)$ approaches zero rapidly as x increases. More specifically, $\mathrm{erfc}(x)$ is asymptotic to

$$u(x) = \exp(-x^2)/(x\sqrt{\pi}) \text{ as } x \to +\infty.$$

For $x > 5$, $\mathrm{erfc}(x)$ satisfies $0.98u(x) < \mathrm{erfc}(x) < u(x)$.



The largest value of x for which $\mathrm{erfc}(x)$ does not underflow is estimated by this subprogram using the System

Parameters subprogram on first entry. Examples of this limiting value, called XMAX in the subprogram, are 9.18 for IEEE single precision and 26.53 for IEEE double precision.

The mathematical function erfce(x) is defined for all x but it is expected to be used only for large positive x. Thus the subprograms SERFCE and DERFCE are designed only for use with $x \geq 0$.

These subprograms are based on polynomial approximations and code due to L. W. Fullerton, Los Alamos, 1977, and rational approximations due to W. J. Cody, [3]. By use of the System Parameters subprogram the accuracy adjusts to the machine precision. The stored coefficients provide for precision to about 30 significant decimal digits for DERF, DERFC, SERF, and SERFC. The accuracy for DERFCE and SERFCE is up to 30 significant decimal digits for $0 \leq x \leq$ XMAX, and up to 18 digits for $x \geq$ XMAX.

Accuracy Tests

The single precision subprograms were tested on a UNISYS 1100 by comparison with the corresponding double precision subprograms at over 45000 points. The relative precision of the UNISYS single precision arithmetic is $\rho = 2^{-27} = 0.745\,\mathrm{E}{-8}$. The test results may be summarized as follows:

Function	Argument Interval	Max. Rel. Error
SERF	$x \leq 1$	2.1ρ
	$x \geq 1$	1.2ρ
SERFC	$[-7, 0.5]$	2.1ρ
	$[0.5, 1.0]$	5.1ρ
	$[1.0, 2.8]$	8ρ
	$[2.8, 4.0]$	16ρ
	$[4.0, 5.7]$	32ρ
	$[5.7, 8.0]$	64ρ
	$[8.0, 8.6]$	128ρ
SERFCE	$[0, 2]$	4ρ
	$[2, 4]$	8ρ
	$[4, 50]$	2ρ

The increase of relative error in SERFC with increasing arguments is an inherent property of the erfc function.

References

1. Milton Abramowitz and Irene A. Stegun, **Handbook of Mathematical Functions**, *Applied Mathematics Series 55*, National Bureau of Standards (1966) Chapter 7, 295–330.

2. J. F. Hart et al., **Computer Approximations**, J. Wiley and Sons, New York (1968) Section 6.7.

3. W. J. Cody, *Rational Chebyshev approximations for the error function*, **Math. of Comp. 23**, 107 (July 1969) 631–637.

E. Error Procedures and Restrictions

The argument for SERFCE or DERFCE must be nonnegative. If it is negative the subprogram will issue an error message and return a zero result.

If the argument for SERFC or DERFC exceeds XMAX, defined above in Section D, the subroutine will issue a warning message and return a zero result.

Error and warning messages are processed using the subroutines of Chapter 19.2 with an error level of zero.

F. Supporting Information

Entry	Required Files
DERF	AMACH, DCSEVL, DERF, DERM1, DERV1, DINITS, ERFIN, ERMSG, IERM1, IERV1
DERFC	AMACH, DCSEVL, DERF, DERM1, DERV1, DINITS, ERFIN, ERMSG, IERM1, IERV1
DERFCE	AMACH, DCSEVL, DERF, DERM1, DERV1, DINITS, ERFIN, ERMSG, IERM1, IERV1
SERF	AMACH, ERFIN, ERMSG, IERM1, IERV1, SCSEVL, SERF, SERM1, SERVI, SINITS
SERFC	AMACH, ERFIN, ERMSG, IERM1, IERV1, SCSEVL, SERF, SERM1, SERVI, SINITS
SERFCE	AMACH, ERFIN, ERMSG, IERM1, IERV1, SCSEVL, SERF, SERM1, SERVI, SINITS

Based on a 1977 program by L. W. Fullerton, Los Alamos, and a 1969 program by E. W. Ng, JPL. Present version by C. L. Lawson and S. Y. Chiu, JPL, 1983.

DRSERF

```
      program DRSERF
c>> 1996-06-17 DRSERF Krogh Minor change in formats for C conversion.
c>> 1994-10-19 DRSERF Krogh  Changes to use M77CON
c>> 1992-05-13 DRSERF CLL
c>> 1991-10-16 DRSERF CLL add demo of SERFCE
c>> 1987-12-09 DRSERF   Lawson   Initial Code.
c--S replaces "?": DR?ERF, ?ERF, ?ERFC, ?ERFCE
c
c     Demonstration driver for SERF, SERFC, and SERFCE
c
      external         R1MACH, SERF, SERFC, SERFCE
      real             R1MACH, SERF, SERFC, SERFCE, X, XMAX, YE, YC, YCE
c
      if(log10(R1MACH(1)) .lt. -65.0e0) then
         XMAX = 12.0e0
      else
         XMAX = 9.0e0
      endif
      X= -6.0E0
      print '(4x,''X'',9x,''SERF'',12x,''SERFC'',10x,''SERFCE''/1x)'
   20 if(X .le. XMAX)then
         YE= SERF(X)
         YC= SERFC(X)
      if(X .lt. 0.0E0)then
            print '(1x,f5.1,1x,2e17.8)', X,YE,YC
      else
            YCE = SERFCE(X)
            print '(1x,f5.1,1x,3e17.8)', X,YE,YC,YCE
      end if
      if(X .lt. 6.0E0)then
            X = X + 0.5E0
      else
            X = X + 1.0E0
      end if
      go to 20
      end if
      stop
      end
```

ODSERF

X	SERF	SERFC	SERFCE
−6.0	−0.10000000E+01	0.20000000E+01	
−5.5	−0.10000000E+01	0.20000000E+01	
−5.0	−0.10000000E+01	0.20000000E+01	
−4.5	−0.10000000E+01	0.20000000E+01	
−4.0	−0.10000000E+01	0.20000000E+01	
−3.5	−0.99999928E+00	0.19999993E+01	
−3.0	−0.99997795E+00	0.19999779E+01	
−2.5	−0.99959302E+00	0.19995930E+01	
−2.0	−0.99532223E+00	0.19953222E+01	
−1.5	−0.96610516E+00	0.19661051E+01	
−1.0	−0.84270078E+00	0.18427007E+01	
−0.5	−0.52049989E+00	0.15204999E+01	
0.0	0.00000000E+00	0.10000000E+01	0.10000000E+01
0.5	0.52049989E+00	0.47950009E+00	0.61569035E+00
1.0	0.84270078E+00	0.15729919E+00	0.42758358E+00
1.5	0.96610516E+00	0.33894852E−01	0.32158542E+00
2.0	0.99532223E+00	0.46777353E−02	0.25539568E+00
2.5	0.99959302E+00	0.40695202E−03	0.21080637E+00
3.0	0.99997795E+00	0.22090497E−04	0.17900115E+00
3.5	0.99999928E+00	0.74309827E−06	0.15529366E+00
4.0	0.10000000E+01	0.15417259E−07	0.13699946E+00
4.5	0.10000000E+01	0.19661604E−09	0.12248480E+00
5.0	0.10000000E+01	0.15374597E−11	0.11070464E+00
5.5	0.10000000E+01	0.73578483E−14	0.10096221E+00
6.0	0.10000000E+01	0.21519734E−16	0.92776567E−01
7.0	0.10000000E+01	0.41838254E−22	0.79800054E−01
8.0	0.10000000E+01	0.11224297E−28	0.69985166E−01
9.0	0.10000000E+01	0.41370317E−36	0.62307723E−01