NAG Library Routine Document

S22BAF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of ***bold italicised*** terms and other implementation-dependent details.

1 Purpose

S22BAF returns a value for the confluent hypergeometric function ${}_1F_1(a;b;x)$ with real parameters a and b, and real argument x. This function is sometimes also known as Kummer's function $M(a,b,x)$.

2 Specification

```
SUBROUTINE S22BAF (A, B, X, M, IFAIL)

INTEGER             IFAIL
REAL (KIND=nag_wp) A, B, X, M
```

3 Description

S22BAF returns a value for the confluent hypergeometric function ${}_1F_1(a;b;x)$ with real parameters a and b, and real argument x. This function is unbounded or not uniquely defined for b equal to zero or a negative integer.

The associated routine S22BBF performs the same operations, but returns M in the scaled form $M = m_f \times 2^{m_s}$ to allow calculations to be performed when M is not representable as a single working precision number. It also accepts the parameters a and b as summations of an integer and a decimal fraction, giving higher accuracy when a or b are close to an integer. In such cases, S22BBF should be used when high accuracy is required.

The confluent hypergeometric function is defined by the confluent series

$$ {}_1F_1(a;b;x) = M(a,b,x) = \sum_{s=0}^{\infty} \frac{(a)_s x^s}{(b)_s s!} = 1 + \frac{a}{b}x + \frac{a(a+1)}{b(b+1)2!}x^2 + \cdots $$

where $(a)_s = 1(a)(a+1)(a+2)\dots(a+s-1)$ is the rising factorial of a. $M(a,b,x)$ is a solution to the second order ODE (Kummer's Equation):

$$ x\frac{d^2M}{dx^2} + (b-x)\frac{dM}{dx} - aM = 0. \quad (1) $$

Given the parameters and argument (a,b,x), this routine determines a set of safe values $\{(\alpha_i,\beta_i,\zeta_i) \mid i \leq 2\}$ and selects an appropriate algorithm to accurately evaluate the functions $M_i(\alpha_i,\beta_i,\zeta_i)$. The result is then used to construct the solution to the original problem $M(a,b,x)$ using, where necessary, recurrence relations and/or continuation.

Additionally, an artificial bound, $arbnd$ is placed on the magnitudes of a, b and x to minimize the occurrence of overflow in internal calculations. $arbnd = 0.0001 \times I_{\max}$, where $I_{\max} = \text{X02BBF}$. It should, however, not be assumed that this routine will produce an accurate result for all values of a, b and x satisfying this criterion.

Please consult the NIST Digital Library of Mathematical Functions or the companion (2010) for a detailed discussion of the confluent hypergeoemtric function including special cases, transformations, relations and asymptotic approximations.

4 References

NIST Handbook of Mathematical Functions (2010) (eds F W J Olver, D W Lozier, R F Boisvert, C W Clark) Cambridge University Press

Pearson J (2009) Computation of hypergeometric functions *MSc Dissertation, Mathematical Institute, University of Oxford*

5 Arguments

1: A – REAL (KIND=nag_wp) *Input*

On entry: the parameter a of the function.

Constraint: $|\mathrm{A}| \leq arbnd$.

2: B – REAL (KIND=nag_wp) *Input*

On entry: the parameter b of the function.

Constraint: $|\mathrm{B}| \leq arbnd$.

3: X – REAL (KIND=nag_wp) *Input*

On entry: the argument x of the function.

Constraint: $|\mathrm{X}| \leq arbnd$.

4: M – REAL (KIND=nag_wp) *Output*

On exit: the solution $M(a,b,x)$.

Note: if overflow occurs upon completion, as indicated by $\mathrm{IFAIL} = 2$, $|M(a,b,x)|$ may be assumed to be too large to be representable. M will be returned as $\pm R_{\mathrm{max}}$, where R_{max} is the largest representable real number (see X02ALF). The sign of M should match the sign of $M(a,b,x)$. If overflow occurs during a subcalculation, as indicated by $\mathrm{IFAIL} = 5$, the sign may be incorrect, and the true value of $M(a,b,x)$ may or may not be greater than R_{max}. In either case it is advisable to subsequently use S22BBF.

5: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this argument, the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

On exit: $\mathrm{IFAIL} = 0$ unless the routine detects an error or a warning has been flagged (see Section 6).

6 Error Indicators and Warnings

If on entry $\mathrm{IFAIL} = 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

$\mathrm{IFAIL} = 1$

Underflow occurred during the evaluation of $M(a,b,x)$.
The returned value may be inaccurate.

IFAIL $= 2$

On completion, overflow occurred in the evaluation of $M(a,b,x)$.

IFAIL $= 3$

All approximations have completed, and the final residual estimate indicates some precision may have been lost.
Relative residual $= \langle value \rangle$.

IFAIL $= 4$

All approximations have completed, and the final residual estimate indicates no accuracy can be guaranteed.
Relative residual $= \langle value \rangle$.

IFAIL $= 5$

Overflow occurred in a subcalculation of $M(a,b,x)$.
The answer may be completely incorrect.

IFAIL $= 11$

On entry, A $= \langle value \rangle$.
Constraint: $|\mathrm{A}| \leq arbnd = \langle value \rangle$.

IFAIL $= 31$

On entry, B $= \langle value \rangle$.
Constraint: $|\mathrm{B}| \leq arbnd = \langle value \rangle$.

IFAIL $= 32$

On entry, B $= \langle value \rangle$.
$M(a,b,x)$ is undefined when b is zero or a negative integer.

IFAIL $= 51$

On entry, X $= \langle value \rangle$.
Constraint: $|\mathrm{X}| \leq arbnd = \langle value \rangle$.

IFAIL $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -399$

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL $= -999$

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

In general, if IFAIL $= 0$, the value of M may be assumed accurate, with the possible loss of one or two decimal places. Assuming the result does not under or overflow, an error estimate res is made internally using equation (1). If the magnitude of res is sufficiently large, a nonzero IFAIL will be returned. Specifically,

IFAIL $= 0$ $\quad res \leq 1000\epsilon$
IFAIL $= 3$ $\quad 1000\epsilon < res \leq 0.1$
IFAIL $= 4$ $\quad res > 0.1$

where ϵ is the ***machine precision*** as returned by X02AJF.

A further estimate of the residual can be constructed using equation (1), and the differential identity,

$$\frac{dM(a,b,x)}{dx} = \frac{a}{b}M(a+1,b+1,x),$$

$$\frac{d^2M(a,b,x)}{dx^2} = \frac{a(a+1)}{b(b+1)}M(a+2,b+2,x).$$

This estimate is however dependent upon the error involved in approximating $M(a+1,b+1,x)$ and $M(a+2,b+2,x)$.

Furthermore, the accuracy of the solution, and the error estimate, can be dependent upon the accuracy of the decimal fraction of the input parameters a and b. For example, if $b = b_i + b_r = 100 + 1.0\text{E}{-6}$, then on a machine with 16 decimal digits of precision, the internal calculation of b_r will only be accurate to 8 decimal places. This can subsequently pollute the final solution by several decimal places without affecting the residual estimate as greatly. Should you require higher accuracy in such regions, then you should use S22BBF, which requires you to supply the correct decimal fraction.

8 Parallelism and Performance

S22BAF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

S22BAF makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

None.

10 Example

This example prints the results returned by S22BAF called using parameters $a = 13.6$ and $b = 14.2$ with 11 differing values of argument x.

10.1 Program Text

```
    Program s22bafe

!     S22BAF Example Program Text

!     Mark 26 Release. NAG Copyright 2016.

!     .. Use Statements ..
      Use nag_library, Only: nag_wp, s22baf
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: a, b, m, x
      Integer                          :: ifail, kx
!     .. Intrinsic Procedures ..
      Intrinsic                        :: real
```

```
!     .. Executable Statements ..
      Write (nout,*) 'S22BAF Example Program Results'

      a = 13.6E0_nag_wp
      b = 14.2E0_nag_wp

      Write (nout,99999) 'a    ', 'b    '
      Write (nout,99998)
      Write (nout,99997) a, b
      Write (nout,99998)
      Write (nout,99994) 'x    ', 'M(a,b,x)  ', 'IFAIL    '
      Write (nout,99995)

      Do kx = -5, 5
        x = real(kx,kind=nag_wp) + 0.5E0_nag_wp
        ifail = -1
        Call s22baf(a,b,x,m,ifail)
        Write (nout,99996) x, m, ifail
      End Do

99999 Format (/,2(1X,A14))
99998 Format (2('+--------------'),'+')
99997 Format (2(1X,F13.2,1X))
99996 Format (1X,F10.2,'    ',1X,E13.5,1X,I9)
99995 Format (3('+--------------'),'+')
99994 Format (/,3(1X,A14))
    End Program s22bafe
```

10.2 Program Data

None.

10.3 Program Results

```
 S22BAF Example Program Results

          a              b
+--------------+--------------+
         13.60          14.20
+--------------+--------------+

          x         M(a,b,x)        IFAIL
+--------------+--------------+--------------+
      -4.50       0.13879E-01         0
      -3.50       0.35674E-01         0
      -2.50       0.92072E-01         0
      -1.50       0.23849E+00         0
      -0.50       0.61969E+00         0
       0.50       0.16148E+01         0
       1.50       0.42184E+01         0
       2.50       0.11045E+02         0
       3.50       0.28978E+02         0
       4.50       0.76166E+02         0
       5.50       0.20053E+03         0
```