NAG Library Routine Document

D01BBF

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.

Note: please be advised that D01BBF has been deprecated and you are advised to use D01TBF.

1 Purpose

D01BBF returns the weights and abscissae appropriate to a Gaussian quadrature formula with a specified number of abscissae. The formulae provided are Gauss–Legendre, rational Gauss, Gauss–Laguerre and Gauss–Hermite.

2 Specification

```
SUBROUTINE D01BBF (D01XXX, A, B, ITYPE, N, WEIGHT, ABSCIS, IFAIL)

INTEGER             ITYPE, N, IFAIL
REAL (KIND=nag_wp) A, B, WEIGHT(N), ABSCIS(N)
EXTERNAL            D01XXX
```

3 Description

D01BBF returns the weights and abscissae for use in the Gaussian quadrature of a function $f(x)$. The quadrature takes the form

$$S = \sum_{i=1}^{n} w_i f(x_i)$$

where w_i are the weights and x_i are the abscissae (see Davis and Rabinowitz (1975), Fröberg (1970), Ralston (1965) or Stroud and Secrest (1966)).

Weights and abscissae are available for Gauss–Legendre, rational Gauss, Gauss–Laguerre and Gauss–Hermite quadrature, and for a selection of values of n (see Section 5).

(a) Gauss–Legendre Quadrature:

$$S \simeq \int_a^b f(x)\,dx$$

where a and b are finite and it will be exact for any function of the form

$$f(x) = \sum_{i=0}^{2n-1} c_i x^i.$$

(b) Rational Gauss quadrature, adjusted weights:

$$S \simeq \int_a^{\infty} f(x)\,dx \qquad (a+b>0) \qquad \text{or} \qquad S \simeq \int_{-\infty}^{a} f(x)\,dx \qquad (a+b<0)$$

and will be exact for any function of the form

$$f(x) = \sum_{i=2}^{2n+1} \frac{c_i}{(x+b)^i} = \frac{\sum_{i=0}^{2n-1} c_{2n+1-i}(x+b)^i}{(x+b)^{2n+1}}.$$

(c) Gauss–Laguerre quadrature, adjusted weights:

$$S \simeq \int_a^{\infty} f(x)\,dx \qquad (b > 0) \qquad \text{or} \qquad S \simeq \int_{-\infty}^{a} f(x)\,dx \qquad (b < 0)$$

and will be exact for any function of the form

$$f(x) = e^{-bx} \sum_{i=0}^{2n-1} c_i x^i.$$

(d) Gauss–Hermite quadrature, adjusted weights:

$$S \simeq \int_{-\infty}^{+\infty} f(x)\,dx$$

and will be exact for any function of the form

$$f(x) = e^{-b(x-a)^2} \sum_{i=0}^{2n-1} c_i x^i \qquad (b > 0).$$

(e) Gauss–Laguerre quadrature, normal weights:

$$S \simeq \int_a^{\infty} e^{-bx} f(x)\,dx \qquad (b > 0) \qquad \text{or} \qquad S \simeq \int_{-\infty}^{a} e^{-bx} f(x)\,dx \qquad (b < 0)$$

and will be exact for any function of the form

$$f(x) = \sum_{i=0}^{2n-1} c_i x^i.$$

(f) Gauss–Hermite quadrature, normal weights:

$$S \simeq \int_{-\infty}^{+\infty} e^{-b(x-a)^2} f(x)\,dx$$

and will be exact for any function of the form

$$f(x) = \sum_{i=0}^{2n-1} c_i x^i.$$

Note: the Gauss–Legendre abscissae, with $a = -1$, $b = +1$, are the zeros of the Legendre polynomials; the Gauss–Laguerre abscissae, with $a = 0$, $b = 1$, are the zeros of the Laguerre polynomials; and the Gauss–Hermite abscissae, with $a = 0$, $b = 1$, are the zeros of the Hermite polynomials.

4 References

Davis P J and Rabinowitz P (1975) *Methods of Numerical Integration* Academic Press

Fröberg C E (1970) *Introduction to Numerical Analysis* Addison–Wesley

Ralston A (1965) *A First Course in Numerical Analysis* pp. 87–90 McGraw–Hill

Stroud A H and Secrest D (1966) *Gaussian Quadrature Formulas* Prentice–Hall

5 Parameters

1: D01XXX – SUBROUTINE, supplied by the NAG Library. *External Procedure*

The name of the routine indicates the quadrature formula:

D01BAZ, for Gauss–Legendre weights and abscissae;

D01BAY, for rational Gauss weights and abscissae;

D01BAX, for Gauss–Laguerre weights and abscissae;

D01BAW, for Gauss–Hermite weights and abscissae.

The name used must be declared as EXTERNAL in the subroutine from which D01BBF is called.

2: A – REAL (KIND=nag_wp) *Input*

3: B – REAL (KIND=nag_wp) *Input*

On entry: the quantities a and b as described in the appropriate sub-section of Section 3.

4: ITYPE – INTEGER *Input*

On entry: indicates the type of weights for Gauss–Laguerre or Gauss–Hermite quadrature (see Section 3).

ITYPE = 1
Adjusted weights will be returned.

ITYPE = 0
Normal weights will be returned.

Constraint: ITYPE = 0 or 1.

For Gauss–Legendre or rational Gauss quadrature, this parameter is not used.

5: N – INTEGER *Input*

On entry: n, the number of weights and abscissae to be returned.

Constraint: N = 1, 2, 3, 4, 5, 6, 8, 10, 12, 14, 16, 20, 24, 32, 48 or 64.

6: WEIGHT(N) – REAL (KIND=nag_wp) array *Output*

On exit: the N weights. For Gauss–Laguerre and Gauss–Hermite quadrature, these will be the adjusted weights if ITYPE = 1, and the normal weights if ITYPE = 0.

7: ABSCIS(N) – REAL (KIND=nag_wp) array *Output*

On exit: the N abscissae.

8: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction 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 parameter, 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: 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 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:

IFAIL = 1

The N-point rule is not among those stored. If the soft fail option is used, the weights and abscissae returned will be those for the largest valid value of N less than the requested value, and the excess elements of WEIGHT and ABSCIS (i.e., up to the requested N) will be filled with zeros.

IFAIL = 2

The value of A and/or B is invalid.

Rational Gauss: $A + B = 0.0$
Gauss–Laguerre: $B = 0.0$
Gauss–Hermite: $B \leq 0.0$

If the soft fail option is used the weights and abscissae are returned as zero.

IFAIL = 3

Laguerre and Hermite normal weights only: underflow is occurring in evaluating one or more of the normal weights. If the soft fail option is used, the underflowing weights are returned as zero. A smaller value of N must be used; or adjusted weights should be used (ITYPE = 1). In the latter case, take care that underflow does not occur when evaluating the integrand appropriate for adjusted weights.

7 Accuracy

The weights and abscissae are stored for standard values of A and B to full machine accuracy.

8 Further Comments

Timing is negligible.

9 Example

This example returns the abscissae and (adjusted) weights for the six-point Gauss–Laguerre formula.

9.1 Program Text

```
    Program d01bbfe

!     D01BBF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: d01bax, d01bbf, nag_wp
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter               :: n = 6, nout = 6
!     .. Local Scalars ..
      Real (Kind=nag_wp)               :: a, b
      Integer                          :: ifail, itype, j
!     .. Local Arrays ..
      Real (Kind=nag_wp)               :: abscis(n), weight(n)
!     .. Executable Statements ..
      Write (nout,*) 'D01BBF Example Program Results'

      a = 0.0E0_nag_wp
      b = 1.0E0_nag_wp
      itype = 1

      ifail = 0
      Call d01bbf(d01bax,a,b,itype,n,weight,abscis,ifail)

      Write (nout,*)
      Write (nout,99998) 'Laguerre formula,', n, ' points'
      Write (nout,*)
      Write (nout,*) '    Abscissae        Weights'
      Write (nout,*)
```

```
      Write (nout,99999)(abscis(j),weight(j),j=1,n)

99999 Format (1X,2E15.6)
99998 Format (1X,A,I3,A)
    End Program d01bbfe
```

9.2 Program Data

None.

9.3 Program Results

```
 D01BBF Example Program Results

 Laguerre formula,  6 points

     Abscissae        Weights

    0.222847E+00   0.573536E+00
    0.118893E+01   0.136925E+01
    0.299274E+01   0.226068E+01
    0.577514E+01   0.335052E+01
    0.983747E+01   0.488683E+01
    0.159829E+02   0.784902E+01
```
