NAG Toolbox

nag_quad_1d_gauss_wset (d01bb)

1 Purpose

nag_quad_1d_gauss_wset (d01bb) 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.

Note: This function is scheduled to be withdrawn, please see d01bb in Advice on Replacement Calls for Withdrawn/Superseded Routines..

2 Syntax

```
[weight, abscis, ifail] = nag_quad_1d_gauss_wset(d01xxx, a, b, itype, n)
[weight, abscis, ifail] = d01bb(d01xxx, a, b, itype, n)
```

3 Description

nag_quad_1d_gauss_wset (d01bb) 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), FrÎberg (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:

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

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:

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

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

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

(e) Gauss–Laguerre quadrature, normal weights:

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

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

FrÎberg 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

5.1 Compulsory Input Parameters

1:

String specifying the quadrature formula to be used:

`'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.

2: **a** – REAL (KIND=nag_wp)
3: **b** – REAL (KIND=nag_wp)

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

4: **itype** – INTEGER

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 argument is not used.

5: **n** – INTEGER

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.

5.2 Optional Input Parameters

None.

5.3 Output Parameters

1: **weight**(**n**) – REAL (KIND=nag_wp) array

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** $= 0$.

2: **abscis**(**n**) – REAL (KIND=nag_wp) array

The **n** abscissae.

3: **ifail** – INTEGER

ifail $= 0$ unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

ifail $= 1$ (*warning*)

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: $\mathbf{a} + \mathbf{b} = 0.0$
Gauss–Laguerre: $\mathbf{b} = 0.0$
Gauss–Hermite: $\mathbf{b} \leq 0.0$

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

ifail $= 3$ (*warning*)

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.

ifail $= -99$

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

ifail $= -399$

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

ifail $= -999$

Dynamic memory allocation failed.

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

```
function d01bb_example

fprintf('d01bb example results\n\n');

a = 0;
b = 1;
itype = nag_int(1);
n = nag_int(6);

[weight, abscis, ifail] = ...
  d01bb( ...
  'd01bax', a, b, itype, n);

fprintf('  Weights    Abscissae\n');
fprintf('%9.4f%12.4f\n',[weight abscis]');
```

9.2 Program Results

```
d01bb example results

  Weights    Abscissae
   0.5735      0.2228
   1.3693      1.1889
   2.2607      2.9927
   3.3505      5.7751
   4.8868      9.8375
   7.8490     15.9829
```