NAG Toolbox

nag_quad_1d_gauss_wres (d01tb)

1 Purpose

nag_quad_1d_gauss_wres (d01tb) returns the weights and abscissae appropriate to a Gaussian quadrature formula with a specified number of abscissae. The formulae provided are for Gauss–Legendre, rational Gauss, Gauss–Laguerre and Gauss–Hermite.

2 Syntax

```
[weight, abscis, ifail] = nag_quad_1d_gauss_wres(key, a, b, n)
[weight, abscis, ifail] = d01tb(key, a, b, n)
```

3 Description

nag_quad_1d_gauss_wres (d01tb) 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:

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

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:

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

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: **key** – INTEGER

Indicates the quadrature formula.

key $= 0$
Gauss–Legendre quadrature on a finite interval, using normal weights.

key $= 3$
Gauss–Laguerre quadrature on a semi-infinite interval, using normal weights.

key $= -3$
Gauss–Laguerre quadrature on a semi-infinite interval, using adjusted weights.

key $= 4$
Gauss–Hermite quadrature on an infinite interval, using normal weights.

key $= -4$
Gauss–Hermite quadrature on an infinite interval, using adjusted weights.

key $= -5$
Rational Gauss quadrature on a semi-infinite interval, using adjusted weights.

Constraint: **key** $= 0$, 3, -3, 4, -4 or -5.

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.

Constraints:

Rational Gauss: $\mathbf{a} + \mathbf{b} \neq 0.0$;
Gauss–Laguerre: $\mathbf{b} \neq 0.0$;
Gauss–Hermite: $\mathbf{b} > 0$.

4: **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.

Note: if $n > 0$ and is not a member of the above list, the maxmium value of n stored below n will be used, and all subsequent elements of **abscis** and **weight** will be returned as zero.

5.2 Optional Input Parameters

None.

5.3 Output Parameters

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

The **n** weights.

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.

ifail $= 2$ (*warning*)

Underflow occurred in calculation of normal weights.

ifail $= 3$ (*warning*)

No nonzero weights were generated for the provided parameters.

ifail $= 11$

Constraint: **key** $= 0,\ 3,\ -3,\ 4,\ -4$ or -5.

ifail $= 12$

The value of **a** and/or **b** is invalid for the chosen **key**. Either:

Constraint: $|\mathbf{a} + \mathbf{b}| > 0.0$.

Constraint: $|\mathbf{b}| > 0.0$.

Constraint: $\mathbf{b} > 0.0$.

ifail $= 14$

Constraint: $\mathbf{n} > 0$.

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 d01tb_example

fprintf('d01tb example results\n\n');

key = nag_int(-3);
a = 0;
b = 1;
n = nag_int(6);

[weight, abscis, ifail] = d01tb( ...
  key, a, b, n);

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

function [fv, iflag, user] = f(x, nx, iflag, user)
  fv = sin(x)./x.*log(10*(1-x));
```

9.2 Program Results

```
 d01tb 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
```