

## NAG C Library Function Document

### nag\_1d\_quad\_wt\_alglog\_1 (d01spc)

#### 1 Purpose

nag\_1d\_quad\_wt\_alglog\_1 (d01spc) is an adaptive integrator which calculates an approximation to the integral of a function  $g(x)w(x)$  over a finite interval  $[a, b]$ :

$$I = \int_a^b g(x)w(x) dx$$

where the weight function  $w$  has end-point singularities of algebraico-logarithmic type.

#### 2 Specification

```
#include <nag.h>
#include <nagd01.h>

void nag_1d_quad_wt_alglog_1 (double (*g)(double x, Nag_User *comm),
                               double a, double b, double alfa, double beta,
                               Nag_QuadWeight wt_func, double epsabs, double epsrel,
                               Integer max_num_subint, double *result, double *abserr,
                               NAG_QuadProgress *qp, Nag_User *comm, NagError *fail)
```

#### 3 Description

This function is based upon the QUADPACK routine QAWSE (Piessens *et al.* (1983)) and integrates a function of the form  $g(x)w(x)$ , where the weight function  $w(x)$  may have algebraico-logarithmic singularities at the end-points  $a$  and/or  $b$ . The strategy is a modification of that in nag\_1d\_quad\_osc\_1 (d01skc). We start by bisecting the original interval and applying modified Clenshaw–Curtis integration of orders 12 and 24 to both halves. Clenshaw–Curtis integration is then used on all sub-intervals which have  $a$  or  $b$  as one of their end-points (Piessens *et al.* (1974)). On the other sub-intervals Gauss–Kronrod (7–15 point) integration is carried out.

A ‘global’ acceptance criterion (as defined by Malcolm and Simpson (1976)) is used. The local error estimation control is described by Piessens *et al.* (1983).

#### 4 Parameters

1:	<b>g</b> – function supplied by user	<i>Function</i>
----	--------------------------------------	-----------------

The function **g**, supplied by the user, must return the value of the function  $g$  at a given point.

The specification of **g** is:

```
double g(double x, Nag_User *comm)
```

1:	<b>x</b> – double	<i>Input</i>
----	-------------------	--------------

*On entry:* the point at which the function  $g$  must be evaluated.

2:   **comm** – Nag\_User \*

*On entry/on exit:* pointer to a structure of type Nag\_User with the following member:

**p** – Pointer

*Input/Output*

*On entry/on exit:* the pointer **comm**→**p** should be cast to the required type, e.g., `struct user *s = (struct user *)comm->p;`, to obtain the original object's address with appropriate type. (See the argument **comm** below.)

2:   **a** – double

*Input*

*On entry:* the lower limit of integration,  $a$ .

3:   **b** – double

*Input*

*On entry:* the upper limit of integration,  $b$ .

*Constraint:*  $\mathbf{b} > \mathbf{a}$ .

4:   **alfa** – double

*Input*

*On entry:* the parameter  $\alpha$  in the weight function.

*Constraint:*  $\mathbf{alfa} > -1.0$ .

5:   **beta** – double

*Input*

*On entry:* the parameter  $\beta$  in the weight function.

*Constraint:*  $\mathbf{beta} > -1.0$ .

6:   **wt\_func** – Nag\_QuadWeight

*Input*

*On entry:* indicates which weight function is to be used:

    if **wt\_func** = Nag\_Alg,  $w(x) = (x - a)^\alpha(b - x)^\beta$ ;

    if **wt\_func** = Nag\_Alg\_loga,  $w(x) = (x - a)^\alpha(b - x)^\beta \ln(x - a)$ ;

    if **wt\_func** = Nag\_Alg\_logb,  $w(x) = (x - a)^\alpha(b - x)^\beta \ln(b - x)$ ;

    if **wt\_func** = Nag\_Alg\_loga\_logb,  $w(x) = (x - a)^\alpha(b - x)^\beta \ln(x - a) \ln(b - x)$ .

*Constraint:* **wt\_func** = Nag\_Alg, Nag\_Alg\_loga, Nag\_Alg\_logb, or Nag\_Alg\_loga\_logb.

7:   **epsabs** – double

*Input*

*On entry:* the absolute accuracy required. If **epsabs** is negative, the absolute value is used. See Section 6.1.

8:   **epsrel** – double

*Input*

*On entry:* the relative accuracy required. If **epsrel** is negative, the absolute value is used. See Section 6.1.

9:   **max\_num\_subint** – Integer

*Input*

*On entry:* the upper bound on the number of sub-intervals into which the interval of integration may be divided by the function. The more difficult the integrand, the larger **max\_num\_subint** should be.

*Suggested values:* a value in the range 200 to 500 is adequate for most problems.

*Constraint:* **max\_num\_subint**  $\geq 2$ .

10:	<b>result</b> – double *	Output
<i>On exit:</i> the approximation to the integral $I$ .		
11:	<b>abserr</b> – double *	Output
<i>On exit:</i> an estimate of the modulus of the absolute error, which should be an upper bound for $ I - \text{result} $ .		
12:	<b>qp</b> – Nag_QuadProgress *	
Pointer to structure of type <b>Nag_QuadProgress</b> with the following members:		
	<b>num_subint</b> – Integer	Output
	<i>On exit:</i> the actual number of sub-intervals used.	
	<b>fun_count</b> – Integer	Output
	<i>On exit:</i> the number of function evaluations performed by nag_1d_quad_wt_alglog_1.	
	<b>sub_int_beg_pts</b> – double *	Output
	<b>sub_int_end_pts</b> – double *	Output
	<b>sub_int_result</b> – double *	Output
	<b>sub_int_error</b> – double *	Output
	<i>On exit:</i> these pointers are allocated memory internally with <b>max_num_subint</b> elements. If an error exit other than <b>NE_INT_ARG_LT</b> , <b>NE_BAD_PARAM</b> , <b>NE_REAL_ARG_LE</b> , <b>NE_2_REAL_ARG_LE</b> or <b>NE_ALLOC_FAIL</b> occurs, these arrays will contain information which may be useful. For details, see Section 6.	
	Before a subsequent call to nag_1d_quad_wt_alglog_1 is made, or when the information contained in these arrays is no longer useful, the user should free the storage allocated by these pointers using the NAG macro <b>NAG_FREE</b> .	
13:	<b>comm</b> – Nag_User *	
	<i>On entry/on exit:</i> pointer to a structure of type <b>Nag_User</b> with the following member:	
	<b>p</b> – Pointer	Input/Output
	<i>On entry/on exit:</i> the pointer <b>p</b> , of type Pointer, allows the user to communicate information to and from the user-defined function <b>g()</b> . An object of the required type should be declared by the user, e.g., a structure, and its address assigned to the pointer <b>p</b> by means of a cast to Pointer in the calling program, e.g., <b>comm.p = (Pointer)&amp;s</b> . The type Pointer is <b>void *</b> .	
14:	<b>fail</b> – NagError *	Input/Output
	The NAG error parameter (see the Essential Introduction).	
	Users are recommended to declare and initialise <b>fail</b> and set <b>fail.print = TRUE</b> for this function.	

## 5 Error Indicators and Warnings

### NE\_INT\_ARG\_LT

On entry, **max\_num\_subint** must not be less than 2: **max\_num\_subint = <value>**.

### NE\_BAD\_PARAM

On entry, parameter **wt\_func** had an illegal value.

**NE\_REAL\_ARG\_LE**

On entry, **alfa** must not be less than or equal to  $-1.0$ : **alfa** = *<value>*.

On entry, **beta** must not be less than or equal to  $-1.0$ : **beta** = *<value>*.

**NE\_2\_REAL\_ARG\_LE**

On entry, **b** = *<value>* while **a** = *<value>*. These parameters must satisfy **b** > **a**.

**NE\_ALLOC\_FAIL**

Memory allocation failed.

**NE\_QUAD\_MAX\_SUBDIV**

The maximum number of subdivisions has been reached: **max\_num\_subint** = *<value>*.

The maximum number of subdivisions has been reached without the accuracy requirements being achieved. Look at the integrand in order to determine the integration difficulties. If the position of a discontinuity or a singularity of algebraico-logarithmic type within the interval can be determined, the interval must be split up at this point and the integrator called on the sub-intervals. If necessary, another integrator, which is designed for handling the type of difficulty involved, must be used. Alternatively, consider relaxing the accuracy requirements specified by **epsabs** and **epsrel**, or increasing the value of **max\_num\_subint**.

**NE\_QUAD\_ROUNDOFF\_TOL**

Round-off error prevents the requested tolerance from being achieved: **epsabs** = *<value>*, **epsrel** = *<value>*.

The error may be underestimated. Consider relaxing the accuracy requirements specified by **epsabs** and **epsrel**.

**NE\_QUAD\_BAD\_SUBDIV**

Extremely bad integrand behaviour occurs around the sub-interval (*<value>*, *<value>*).

The same advice applies as in the case of **NE\_QUAD\_MAX\_SUBDIV**.

## 6 Further Comments

The time taken by nag\_1d\_quad\_wt\_alglog\_1 depends on the integrand and the accuracy required.

If the function fails with an error exit other than **NE\_INT\_ARG\_LT**, **NE\_BAD\_PARAM**, **NE\_REAL\_ARG\_LE**, **NE\_2\_REAL\_ARG\_LE** or **NE\_ALLOC\_FAIL** then the user may wish to examine the contents of the structure **qp**. These contain the end-points of the sub-intervals used by nag\_1d\_quad\_wt\_alglog\_1 along with the integral contributions and error estimates over these sub-intervals.

Specifically, for  $i = 1, 2, \dots, n$ , let  $r_i$  denote the approximation to the value of the integral over the sub-interval  $[a_i, b_i]$  in the partition of  $[a, b]$  and  $e_i$  be the corresponding absolute error estimate.

Then,  $\int_{a_i}^{b_i} g(x)w(x) dx \simeq r_i$  and **result** =  $\sum_{i=1}^n r_i$ .

The value of  $n$  is returned in **num\_subint**, and the values  $a_i$ ,  $b_i$ ,  $r_i$  and  $e_i$  are stored in the structure **qp** as

$a_i = \text{sub\_int\_beg\_pts}[i - 1]$ ,

$b_i = \text{sub\_int\_end\_pts}[i - 1]$ ,

$r_i = \text{sub\_int\_result}[i - 1]$  and

$e_i = \text{sub\_int\_error}[i - 1]$ .

## 6.1 Accuracy

The function cannot guarantee, but in practice usually achieves, the following accuracy:

$$|I - \text{result}| \leq tol$$

where

$$tol = \max\{|\text{epsabs}|, |\text{epsrel}| \times |I|\}$$

and **epsabs** and **epsrel** are user-specified absolute and relative error tolerances. Moreover it returns the quantity **abserr** which, in normal circumstances, satisfies

$$|I - \text{result}| \leq \text{abserr} \leq tol.$$

## 6.2 References

Malcolm M A and Simpson R B (1976) Local versus global strategies for adaptive quadrature *ACM Trans. Math. Software* **1** 129–146

Piessens R, Mertens I and Branders M (1974) Integration of functions having end-point singularities *Angew. Inf.* **16** 65–68

Piessens R, De Doncker-Kapenga E, Überhuber C and Kahaner D (1983) *QUADPACK, A Subroutine Package for Automatic Integration* Springer-Verlag

## 7 See Also

nag\_1d\_quad\_gen\_1 (d01sjc)

## 8 Example

To compute

$$\int_0^1 \ln x \cos(10\pi x) dx$$

and

$$\int_0^1 \frac{\sin(10x)}{\sqrt{x(1-x)}} dx.$$

### 8.1 Program Text

```
/* nag_1d_quad_wt_alglog_1(d01spc) Example Program
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 * Mark 6 revised, 2000.
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdl�.h>
#include <math.h>
#include <nagd01.h>
#include <nagx01.h>

static double f_sin(double x, Nag_User *comm);
static double f_cos(double x, Nag_User *comm);
```

```

main()
{
    static double alfa[2] = {0.0, -0.5};
    static double beta[2] = {0.0, -0.5};
    Nag_QuadWeight wt_func;
    double a, b;
    double epsabs, abserr, epsrel, result;
    static NagError fail;
    Nag_QuadProgress qp;
    Integer max_num_subint;
    int numfunc;
    NAG_D01SPC_FUN g;
    static char *Nag_QuadWeight_array[] =
    { "Nag_Alg", "Nag_Alg_loga", "Nag_Alg_logb", "Nag_Alg_loga_logb" };
    Boolean success = TRUE;
    Nag_User comm;
    Integer wt_array_ind;

    Vprintf("d01spc Example Program Results\n");
    epsabs = 0.0;
    epsrel = 0.0001;
    a = 0.0;
    b = 1.0;
    max_num_subint = 200;
    for (numfunc=0; numfunc < 2; ++numfunc)
    {
        switch (numfunc)
        {
        case 0:
            g = f_cos;
            wt_func = Nag_Alg_loga;
            wt_array_ind = 1;
            break;
        case 1:
            g = f_sin;
            wt_func = Nag_Alg;
            wt_array_ind = 0;
        }
        d01spc(g, a, b, alfa[numfunc], beta[numfunc],
                wt_func, epsabs, epsrel, max_num_subint,
                &result, &abserr, &qp, &comm, &fail);

        Vprintf("a      - lower limit of integration = %10.4f\n", a);
        Vprintf("b      - upper limit of integration = %10.4f\n", b);
        Vprintf("epsabs - absolute accuracy requested = %9.2e\n", epsabs);
        Vprintf("epsrel - relative accuracy requested = %9.2e\n", epsrel);
        Vprintf("alfa   - parameter in the weight function = %10.4f\n",
               alfa[numfunc]);
        Vprintf("beta   - parameter in the weight function = %10.4f\n",
               beta[numfunc]);
        Vprintf("wt_func - denotes weight function to be \
used = %s\n", Nag_QuadWeight_array[wt_array_ind]);
        if (fail.code != NE_NOERROR)
            Vprintf("%s\n", fail.message);
        if (fail.code != NE_INT_ARG_LT && fail.code != NE_BAD_PARAM &&
            fail.code != NE_REAL_ARG_LE && fail.code != NE_2_REAL_ARG_LE &&
            fail.code != NE_ALLOC_FAIL)

```

```

    {
        Vprintf("result - approximation to the integral = %9.5f\n", result);
        Vprintf("abserr - estimate of the absolute error = %9.2e\n", abserr);
        Vprintf("qp.fun_count - number of function evaluations = %4ld\n",
                qp.fun_count);
        Vprintf("qp.num_subint - number of subintervals used = %4ld\n\n",
                qp.num_subint);
        /* Free memory used by qp */
        NAG_FREE(qp.sub_int_beg_pts);
        NAG_FREE(qp.sub_int_end_pts);
        NAG_FREE(qp.sub_int_result);
        NAG_FREE(qp.sub_int_error);
    }
    else
        success = FALSE;
}
if (success)
    exit(EXIT_SUCCESS);
else
    exit(EXIT_FAILURE);
}

static double f_cos(double x, Nag_User *comm)
{
    double a;
    double pi;

    pi = X01AAC;
    a = pi*10.0;
    return cos(a*x);
}

static double f_sin(double x, Nag_User *comm)
{
    double omega;

    omega = 10.0;
    return sin(omega*x);
}

```

## 8.2 Program Data

None.

## 8.3 Program Results

```

d01spc Example Program Results
a      - lower limit of integration =      0.0000
b      - upper limit of integration =      1.0000
epsabs - absolute accuracy requested =  0.00e+00
epsrel - relative accuracy requested =  1.00e-04

alfa   - parameter in the weight function =      0.0000
beta   - parameter in the weight function =      0.0000
wt_func - denotes weight function to be used = Nag_Alg_loga
result - approximation to the integral = -0.04899
abserr - estimate of the absolute error =  1.14e-07
qp.fun_count - number of function evaluations = 110

```

```
qp.num_subint - number of subintervals used =      4
a      - lower limit of integration =      0.0000
b      - upper limit of integration =      1.0000
epsabs - absolute accuracy requested =  0.00e+00
epsrel - relative accuracy requested =  1.00e-04

alfa   - parameter in the weight function =      -0.5000
beta   - parameter in the weight function =      -0.5000
wt_func - denotes weight function to be used = Nag_Alg
result - approximation to the integral =      0.53502
abserr - estimate of the absolute error =  1.94e-12
qp.fun_count - number of function evaluations =    50
qp.num_subint - number of subintervals used =      2
```

---