

NAG 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

nag_1d_quad_wt_alglog_1 (d01spc) 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 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, de Doncker–Kapenga E, Überhuber C and Kahaner D (1983) *QUADPACK, A Subroutine Package for Automatic Integration* Springer–Verlag
- Piessens R, Mertens I and Branders M (1974) Integration of functions having end-point singularities *Angew. Inf.* **16** 65–68

5 Arguments

- 1: **g** – function, supplied by the user *External Function*
g 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: **x** – double *Input*

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

2: **comm** – Nag_User *

Pointer to a structure of type Nag_User with the following member:

p – Pointer

On entry/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: **b** > **a**.

- 4: **alfa** – double *Input*
On entry: the argument α in the weight function.
Constraint: **alfa** > -1.0.

- 5: **beta** – double *Input*
On entry: the argument β in the weight function.
Constraint: **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 7.

- 8: **epsrel** – double *Input*
On entry: the relative accuracy required. If **epsrel** is negative, the absolute value is used. See Section 7.
- 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.
Constraint: **max_num_subint** ≥ 2 .
- 10: **result** – double * *Output*
On exit: the approximation to the integral I .
- 11: **abserr** – double * *Output*
On exit: an estimate of the modulus of the absolute error, which should be an upper bound for $|I - \mathbf{result}|$.
- 12: **qp** – Nag_QuadProgress *
 Pointer to structure of type Nag_QuadProgress with the following members:
- num_subint** – Integer *Output*
On exit: the actual number of sub-intervals used.
- fun_count** – Integer *Output*
On exit: the number of function evaluations performed by nag_1d_quad_wt_alglog_1 (d01spc).
- sub_int_beg_pts** – double * *Output*
sub_int_end_pts – double * *Output*
sub_int_result – double * *Output*
sub_int_error – double * *Output*
- On exit:* these pointers are allocated memory internally with **max_num_subint** elements. If 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 occurs, these arrays will contain information which may be useful. For details, see Section 9.
- Before a subsequent call to nag_1d_quad_wt_alglog_1 (d01spc) is made, or when the information contained in these arrays is no longer useful, you should free the storage allocated by these pointers using the NAG macro NAG_FREE.
- 13: **comm** – Nag_User *
 Pointer to a structure of type Nag_User with the following member:
- p** – Pointer
On entry/exit: the pointer **comm**→**p**, of type Pointer, allows you to communicate information to and from **g()**. An object of the required type should be declared, e.g., a structure, and its address assigned to the pointer **comm**→**p** by means of a cast to Pointer in the calling program, e.g., **comm.p** = (Pointer)&**s**. The type Pointer is void *.
- 14: **fail** – NagError * *Input/Output*
 The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_2_REAL_ARG_LE

On entry, $\mathbf{b} = \langle value \rangle$ while $\mathbf{a} = \langle value \rangle$. These arguments must satisfy $\mathbf{b} > \mathbf{a}$.

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

On entry, argument **wt_func** had an illegal value.

NE_INT_ARG_LT

On entry, **max_num_subint** must not be less than 2: **max_num_subint** = $\langle value \rangle$.

NE_QUAD_BAD_SUBDIV

Extremely bad integrand behaviour occurs around the sub-interval $(\langle value \rangle, \langle value \rangle)$. The same advice applies as in the case of NE_QUAD_MAX_SUBDIV.

NE_QUAD_MAX_SUBDIV

The maximum number of subdivisions has been reached: **max_num_subint** = $\langle value \rangle$.

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** = $\langle value \rangle$, **epsrel** = $\langle value \rangle$.

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

NE_REAL_ARG_LE

On entry, **alfa** = $\langle value \rangle$.

Constraint: **alfa** ≤ -1.0 .

On entry, **beta** = $\langle value \rangle$.

Constraint: **beta** ≤ -1.0 .

7 Accuracy

nag_1d_quad_wt_alglog_1 (d01spc) cannot guarantee, but in practice usually achieves, the following accuracy:

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

where $tol = \max\{|\mathbf{epsabs}|, |\mathbf{epsrel}| \times |I|\}$ and **epsabs** and **epsrel** are user-specified absolute and relative error tolerances. Moreover it returns the quantity **abserr** which, in normal circumstances, satisfies

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

8 Parallelism and Performance

Not applicable.

9 Further Comments

The time taken by `nag_1d_quad_wt_alglog_1` (d01spc) 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 you 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` (d01spc) along with the integral contributions and error estimates over these sub-intervals.

Specifically, $i = 1, 2, \dots, n$, 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 $\mathbf{result} = \sum_{i=1}^n r_i$.

The value of n is returned in `qp`→`num_subint`, and the values a_i , b_i , r_i and e_i are stored in the structure `qp` as

```

a_i = qp→sub_int_beg_pts[i - 1],
b_i = qp→sub_int_end_pts[i - 1],
r_i = qp→sub_int_result[i - 1] and
e_i = qp→sub_int_error[i - 1].

```

10 Example

This example computes

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

and

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

10.1 Program Text

```

/* nag_1d_quad_wt_alglog_1 (d01spc) Example Program.
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 * Mark 6 revised, 2000.
 * Mark 7 revised, 2001.
 *
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagd01.h>
#include <nagx01.h>

#ifdef __cplusplus
extern "C" {
#endif
static double NAG_CALL f_sin(double x, Nag_User *comm);

```

```

static double NAG_CALL f_cos(double x, Nag_User *comm);
#ifdef __cplusplus
}
#endif

int main(void)
{
    /* Scalars */
    Integer      exit_status = 0;
    Integer      max_num_subint, wt_array_ind;
    int          numfunc;
    double       a, b, epsabs, abserr, epsrel, result;
    /* Arrays */
    static Integer use_comm[2] = {1, 1};
    static double  alpha[2] = { 0.0, -0.5 };
    static double  beta[2] = { 0.0, -0.5 };
    static const char *Nag_QuadWeight_array[] = { "Nag_Alq", "Nag_Alq_log",
    "Nag_Alq_logb", "Nag_Alq_logb" };

    /* Nag Types */
    Nag_QuadProgress qp;
    Nag_QuadWeight  wt_func;
    Nag_User        comm;
    NagError        fail;

    INIT_FAIL(fail);

    printf("nag_ld_quad_wt_alglog_1 (d01spc) Example Program Results\n");

    /* For communication with user-supplied functions: */
    comm.p = (Pointer)

    epsabs = 0.0;
    epsrel = 0.0001;
    a = 0.0;
    b = 1.0;
    max_num_subint = 200;
    for (numfunc = 0; numfunc < 2; ++numfunc)
    {
        switch (numfunc)
        {
            default:
            case 0:
                wt_func = Nag_Alq_log;
                wt_array_ind = 1;
                /* nag_ld_quad_wt_alglog_1 (d01spc).
                * One-dimensional adaptive quadrature, weight function with
                * end-point singularities of algebraic-logarithmic type,
                * thread-safe
                */
                nag_ld_quad_wt_alglog_1(f_cos, a, b, alpha[numfunc], beta[numfunc],
                wt_func, epsabs, epsrel, max_num_subint,
                &result, &abserr, &qp, &comm, &fail);
                printf("\nIntegral of cos(10*pi*x) on [a,b]\n");
                break;
            case 1:
                wt_func = Nag_Alq;
                wt_array_ind = 0;
                nag_ld_quad_wt_alglog_1(f_sin, a, b, alpha[numfunc], beta[numfunc],
                wt_func, epsabs, epsrel, max_num_subint,
                &result, &abserr, &qp, &comm, &fail);
                printf("\nIntegral of sin(10*x) on [a,b]\n");
        }
        printf("-----\n");
        printf("a          - lower limit of integration      = %9.4f\n", a);
        printf("b          - upper limit of integration          = %9.4f\n", b);
        printf("epsabs    - absolute accuracy requested          = %11.2e\n", epsabs);
        printf("epsrel    - relative accuracy requested          = %11.2e\n\n", epsrel);
        printf("alpha     - weight function parameter            = %9.4f\n",
        alpha[numfunc]);
        printf("beta     - weight function parameter            = %9.4f\n",
        beta[numfunc]);
    }
}

```

```

printf("wt_func - weight function used          = %s\n",
      Nag_QuadWeight_array[wt_array_ind]);

if (fail.code != NE_NOERROR) printf("%s\n", fail.message);

if (fail.code == NE_NOERROR || fail.code == NE_QUAD_BAD_SUBDIV ||
    fail.code == NE_QUAD_MAX_SUBDIV || fail.code == NE_QUAD_ROUNDOFF_TOL)
{
    printf("result - approximation to the integral = %10.5f\n",
          result);
    printf("abserr - estimate of absolute error   = %11.2e\n",
          abserr);
    printf("qp.fun_count - function evaluations   = %4ld\n",
          qp.fun_count);
    printf("qp.num_subint - 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
{
    exit_status = 1;
    goto END;
}
}

END:
return exit_status;
}

```

```

static double NAG_CALL f_cos(double x, Nag_User *comm)
{
    double a;
    double pi;
    Integer *use_comm = (Integer *)comm->p;

    if (use_comm[0])
    {
        printf("(User-supplied callback f_cos, first invocation.)\n");
        use_comm[0] = 0;
    }

    /* nag_pi (x01aac). */
    pi = nag_pi;
    a = pi*10.0;
    return cos(a*x);
}

```

```

static double NAG_CALL f_sin(double x, Nag_User *comm)
{
    double omega;
    Integer *use_comm = (Integer *)comm->p;

    if (use_comm[1])
    {
        printf("(User-supplied callback f_sin, first invocation.)\n");
        use_comm[1] = 0;
    }

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

```

10.2 Program Data

None.

10.3 Program Results

nag_ld_quad_wt_alglog_1 (d01spc) Example Program Results
(User-supplied callback f_cos, first invocation.)

Integral of $\cos(10\pi x)$ on [a,b]

```
-----
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

alpha  - weight function parameter    = 0.0000
beta   - weight function parameter    = 0.0000
wt_func - weight function used         = Nag_Alq_logq
result - approximation to the integral = -0.04899
abserr - estimate of absolute error    = 1.14e-07
qp.fun_count - function evaluations    = 110
qp.num_subint - subintervals used     = 4
```

(User-supplied callback f_sin, first invocation.)

Integral of $\sin(10x)$ on [a,b]

```
-----
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

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