

# NAG Library Function Document

## nag\_1d\_quad\_inf\_1 (d01smc)

### 1 Purpose

nag\_1d\_quad\_inf\_1 (d01smc) calculates an approximation to the integral of a function  $f(x)$  over an infinite or semi-infinite interval  $[a, b]$ :

$$I = \int_a^b f(x) dx.$$

### 2 Specification

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

void nag_1d_quad_inf_1 (
    double (*f)(double x, Nag_User *comm),
    Nag_BoundInterval boundinf, double bound, double epsabs, double epsrel,
    Integer max_num_subint, double *result, double *abserr,
    Nag_QuadProgress *qp, Nag_User *comm, Nag_Error *fail)
```

### 3 Description

nag\_1d\_quad\_inf\_1 (d01smc) is based on the QUADPACK routine QAGI (Piessens *et al.* (1983)). The entire infinite integration range is first transformed to  $[0, 1]$  using one of the identities

$$\begin{aligned} \int_{-\infty}^a f(x) dx &= \int_0^1 f\left(a - \frac{1-t}{t}\right) \frac{1}{t^2} dt \\ \int_a^{\infty} f(x) dx &= \int_0^1 f\left(a + \frac{1-t}{t}\right) \frac{1}{t^2} dt \\ \int_{-\infty}^{\infty} f(x) dx &= \int_0^1 (f(x) + f(-x)) dx = \int_0^1 \left[ f\left(\frac{1-t}{t}\right) + f\left(\frac{-1+t}{t}\right) \right] \frac{1}{t^2} dt \end{aligned}$$

where  $a$  represents a finite integration limit. An adaptive procedure, based on the Gauss 7-point and Kronrod 15-point rules, is then employed on the transformed integral. The algorithm, described by de Doncker (1978), incorporates a global acceptance criterion (as defined by Malcolm and Simpson (1976)) together with the  $\epsilon$ -algorithm (Wynn (1956)) to perform extrapolation. The local error estimation is described by Piessens *et al.* (1983).

### 4 References

de Doncker E (1978) An adaptive extrapolation algorithm for automatic integration *ACM SIGNUM Newsl.* **13**(2) 12–18

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

Wynn P (1956) On a device for computing the  $e_m(S_n)$  transformation *Math. Tables Aids Comput.* **10** 91–96

## 5 Arguments

- 1: **f** – function, supplied by the user *External Function*  
**f** must return the value of the integrand  $f$  at a given point.

The specification of **f** is:

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

- 1: **x** – double *Input*

*On entry:* the point at which the integrand  $f$  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: **boundinf** – Nag\_BoundInterval *Input*

*On entry:* indicates the kind of integration interval.

**boundinf** = Nag\_UpperSemiInfinite

The interval is  $[\mathbf{bound}, +\infty)$ .

**boundinf** = Nag\_LowerSemiInfinite

The interval is  $(-\infty, \mathbf{bound}]$ .

**boundinf** = Nag\_Infinite

The interval is  $(-\infty, +\infty)$ .

*Constraint:* **boundinf** = Nag\_UpperSemiInfinite, Nag\_LowerSemiInfinite or Nag\_Infinite.

- 3: **bound** – double *Input*

*On entry:* the finite limit of the integration interval (if present). **bound** is not used if **boundinf** = Nag\_Infinite.

- 4: **epsabs** – double *Input*

*On entry:* the absolute accuracy required. If **epsabs** is negative, the absolute value is used. See Section 7.

- 5: **epsrel** – double *Input*

*On entry:* the relative accuracy required. If **epsrel** is negative, the absolute value is used. See Section 7.

- 6: **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**  $\geq 1$ .

- 7: **result** – double \* *Output*

*On exit:* the approximation to the integral  $I$ .

- 8:    **abserr** – double \* *Output*  
*On exit:* an estimate of the modulus of the absolute error, which should be an upper bound for  $|I - \text{result}|$ .
- 9:    **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\_inf\_1 (d01smc).
- 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 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\_inf\_1 (d01smc) 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.
- 10:   **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 **f()**. 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 \*.
- 11:   **fail** – NagError \* *Input/Output*  
 The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

### NE\_BAD\_PARAM

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

### NE\_INT\_ARG\_LT

On entry, **max\_num\_subint** must not be less than 1: **max\_num\_subint** =  $\langle \text{value} \rangle$ .

### NE\_QUAD\_BAD\_SUBDIV

Extremely bad integrand behaviour occurs around the sub-interval  $(\langle \text{value} \rangle, \langle \text{value} \rangle)$ . The same advice applies as in the case of NE\_QUAD\_MAX\_SUBDIV.

**NE\_QUAD\_BAD\_SUBDIV\_INTS**

Extremely bad integrand behaviour occurs around one of the sub-intervals ( $\langle value \rangle$ ,  $\langle value \rangle$ ) or ( $\langle value \rangle$ ,  $\langle value \rangle$ ).

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 local difficulty within the interval can be determined (e.g., a singularity of the integrand or its derivative, a peak, a discontinuity, etc.) you will probably gain from splitting up the interval at this point and calling the integrator 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\_NO\_CONV**

The integral is probably divergent or slowly convergent.

Please note that divergence can also occur with any error exit other than NE\_INT\_ARG\_LT, NE\_BAD\_PARAM or NE\_ALLOC\_FAIL.

**NE\_QUAD\_ROUNDOff\_EXTRAPL**

Round-off error is detected during extrapolation.

The requested tolerance cannot be achieved, because the extrapolation does not increase the accuracy satisfactorily; the returned result is the best that can be obtained.

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

**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**.

**7 Accuracy**

nag\_1d\_quad\_inf\_1 (d01smc) 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

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

**8 Parallelism and Performance**

nag\_1d\_quad\_inf\_1 (d01smc) is not threaded in any implementation.

**9 Further Comments**

The time taken by nag\_1d\_quad\_inf\_1 (d01smc) 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` 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_ld_quad_inf_1` (d01smc) along with the integral contributions and error estimates over the 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,  $\int_{a_i}^{b_i} f(x)dx \simeq r_i$  and **result** =  $\sum_{i=1}^n r_i$  unless the function terminates while testing for divergence of the integral (see Section 3.4.3 of Piessens *et al.* (1983)). In this case, **result** (and **abserr**) are taken to be the values returned from the extrapolation process. 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

```

ai = qp→sub_int_beg_pts[i - 1],
bi = qp→sub_int_end_pts[i - 1],
ri = qp→sub_int_result[i - 1] and
ei = qp→sub_int_error[i - 1].

```

## 10 Example

This example computes

$$\int_0^{\infty} \frac{1}{(x+1)\sqrt{x}} dx.$$

### 10.1 Program Text

```

/* nag_ld_quad_inf_1 (d01smc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

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

int main(void)
{
    static Integer use_comm[1] = { 1 };
    Integer exit_status = 0;
    double a;
    double epsabs, abserr, epsrel, result;
    Nag_QuadProgress qp;
    Integer max_num_subint;
    NagError fail;
    Nag_User comm;

    INIT_FAIL(fail);

```

```

printf("nag_ld_quad_inf_1 (d01smc) Example Program Results\n");

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

epsabs = 0.0;
epsrel = 0.0001;
a = 0.0;
max_num_subint = 200;

/* nag_ld_quad_inf_1 (d01smc).
 * One-dimensional adaptive quadrature over infinite or
 * semi-infinite interval, thread-safe
 */
nag_ld_quad_inf_1(f, Nag_UpperSemiInfinite, a, epsabs, epsrel,
                  max_num_subint, &result, &abserr, &qp, &comm, &fail);
printf("a      - lower limit of integration = %10.4f\n", a);
printf("b      - upper limit of integration = infinity\n");
printf("epsabs - absolute accuracy requested = %11.2e\n", epsabs);
printf("epsrel - relative accuracy requested = %11.2e\n\n", epsrel);
if (fail.code != NE_NOERROR)
    printf("Error from nag_ld_quad_inf_1 (d01smc)  %s\n", fail.message);
if (fail.code != NE_INT_ARG_LT && fail.code != NE_BAD_PARAM &&
    fail.code != NE_ALLOC_FAIL && fail.code != NE_NO_LICENCE) {
    printf("result - approximation to the integral = %9.5f\n", result);
    printf("abserr - estimate of the absolute error = %11.2e\n", abserr);
    printf("qp.fun_count - number of function evaluations = %4" NAG_IFMT
          "\n", qp.fun_count);
    printf("qp.num_subint - number of subintervals used = %4" NAG_IFMT "\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(double x, Nag_User *comm)
{
    Integer *use_comm = (Integer *) comm->p;

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

    return 1.0 / ((x + 1.0) * sqrt(x));
}

```

## 10.2 Program Data

None.

## 10.3 Program Results

```

nag_ld_quad_inf_1 (d01smc) Example Program Results
(User-supplied callback f, first invocation.)
a      - lower limit of integration =      0.0000
b      - upper limit of integration = infinity
epsabs - absolute accuracy requested =      0.00e+00
epsrel - relative accuracy requested =      1.00e-04

```

```
result - approximation to the integral = 3.14159
abserr - estimate of the absolute error = 2.65e-05
qp.fun_count - number of function evaluations = 285
qp.num_subint - number of subintervals used = 10
```

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