

# NAG C Library Function Document

## nag\_1d\_quad\_gen (d01ajc)

### 1 Purpose

nag\_1d\_quad\_gen (d01ajc) is a general purpose integrator which calculates an approximation to the integral of a function  $f(x)$  over a finite interval  $[a, b]$ :

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

### 2 Specification

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

void nag_1d_quad_gen (double (*f)(double x),
                     double a, double b, double epsabs, double epsrel,
                     Integer max_num_subint, double *result, double *abserr,
                     Nag_QuadProgress *qp, NagError *fail)
```

### 3 Description

This function is based upon the QUADPACK routine QAGS (Piessens *et al.* (1983)). It is an adaptive function, using the Gauss 10-point and Kronrod 21-point rules. 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).

The function is suitable as a general purpose integrator, and can be used when the integrand has singularities, especially when these are of algebraic or logarithmic type.

This function requires the user to supply a function to evaluate the integrand at a single point.

### 4 Parameters

1: **f** – function supplied by user *Function*

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

The specification of **f** is:

double f(double x)	
1: <b>x</b> – double	<i>Input</i>
<i>On entry:</i> the point at which the integrand $f$ must be evaluated.	

2: **a** – double *Input*

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

3: **b** – double *Input*

*On entry:* the upper limit of integration,  $b$ . It is not necessary that  $a < b$ .

4: **epsabs** – double *Input*

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

- 5: **epsrel** – double *Input*  
*On entry:* the relative accuracy required. If **epsrel** is negative, the absolute value is used. See Section 6.1.
- 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.  
*Suggested values:* a value in the range 200 to 500 is adequate for most problems.  
*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\_gen.
- 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** or **NE\_ALLOC\_FAIL** occurs, these arrays will contain information which may be useful. For details, see Section 6.
- Before a subsequent call to nag\_1d\_quad\_gen 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 **NAG\_FREE**.
- 10: **fail** – NagError \* *Input/Output*  
 The NAG error parameter (see the Essential Introduction).  
 Users are recommended to declare and initialise **fail** and set **fail.print = TRUE** for this function.

## 5 Error Indicators and Warnings

### NE\_INT\_ARG\_LT

On entry, **max\_num\_subint** must not be less than 1: **max\_num\_subint** = *<value>*.

### 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 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\_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**.

**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\_NO\_CONV**

The integral is probably divergent or slowly convergent.

Please note that divergence can occur with any error exit other than **NE\_INT\_ARG\_LT** and **NE\_ALLOC\_FAIL**.

**6 Further Comments**

The time taken by `nag_1d_quad_gen` depends on the integrand and the accuracy required.

If the function fails with an error exit other than **NE\_INT\_ARG\_LT** 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_gen` along with the integral contributions and error estimates over the 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,  $\int_{a_i}^{b_i} f(x) dx \simeq r_i$  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 **num\_subint**, and the values  $a_i$ ,  $b_i$ ,  $r_i$  and  $e_i$  are stored in the structure **qp** as

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

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

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

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

## 6.1 Accuracy

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

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

where

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

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

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

## 6.2 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

## 7 See Also

nag\_1d\_quad\_osc (d01akc)  
nag\_1d\_quad\_brkpts (d01alc)

## 8 Example

To compute

$$\int_0^{2\pi} \frac{x \sin(30x)}{\sqrt{\left(1 - \left(\frac{x}{2\pi}\right)^2\right)}} dx.$$

### 8.1 Program Text

```
/* nag_1d_quad_gen(d01ajc) Example Program
 *
 * Copyright 1991 Numerical Algorithms Group.
 *
 * Mark 2, 1991.
 *
 * Mark 6 revised, 2000.
 */
```

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

static double f(double x);

main()
```

```

{
  double a, b;
  double epsabs, abserr, epsrel, result;
  Nag_QuadProgress qp;
  Integer max_num_subint;
  static NagError fail;
  double pi = X01AAC;

  Vprintf("d01ajc Example Program Results\n");
  epsabs = 0.0;
  epsrel = 0.0001;
  a = 0.0;
  b = pi*2.0;
  max_num_subint = 200;
  d01ajc(f, a, b, epsabs, epsrel, max_num_subint, &result, &abserr,
        &qp, &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\n", epsrel);
  if (fail.code != NE_NOERROR)
    Vprintf("%s\n", fail.message);
  if (fail.code != NE_INT_ARG_LT && 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",
            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);
      exit(EXIT_SUCCESS);
    }
  else
    exit(EXIT_FAILURE);
}

static double f(double x)
{
  double pi = X01AAC;
  return (x*sin(x*30.0)/sqrt(1.0-x*x/(pi*pi*4.0)));
}

```

## 8.2 Program Data

None.

### 8.3 Program Results

```
d01ajc Example Program Results
a      - lower limit of integration =    0.0000
b      - upper limit of integration =    6.2832
epsabs - absolute accuracy requested =  0.00e+00
epsrel - relative accuracy requested =  1.00e-04

result - approximation to the integral = -2.54326
abserr - estimate of the absolute error =  1.28e-05
qp.fun_count - number of function evaluations =  777
qp.num_subint - number of subintervals used =   19
```

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