

NAG C Library Function Document

nag_1d_quad_gen_1 (d01sjc)

1 Purpose

nag_1d_quad_gen_1 (d01sjc) 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_1 (double (*f)(double x, Nag_User *comm),
                       double a, double b, 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 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 ϵ -algorithm (Wynn (1956)) to perform extrapolation. The local error estimation is described by Piessens *et al.* (1983).

This 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, Nag_User *comm) | |
| 1: | x – double <i>Input</i> |
| | <i>On entry:</i> the point at which the integrand f must be evaluated. |
| 2: | comm – Nag_User * |
| | <i>On entry/on exit:</i> pointer to a structure of type Nag_User with the following member: |
| | p – Pointer <i>Input/Output</i> |
| | <i>On entry/on exit:</i> 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*. 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: $\text{max_num_subint} \geq 1$.
- 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_1`.
- sub_int_be_pts_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_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 **NAG_FREE**.

10: **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 **p**, of type Pointer, allows the user to communicate information to and from the user-defined function **f()**. An object of the required type should be declared by the user, e.g., a structure, and its address assigned to the pointer **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 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_1` 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_1` 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

$$\begin{aligned} a_i &= \text{sub_int_beg_pts}[i - 1], \\ b_i &= \text{sub_int_end_pts}[i - 1], \\ r_i &= \text{sub_int_result}[i - 1] \text{ and} \\ e_i &= \text{sub_int_error}[i - 1]. \end{aligned}$$

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_1` (d01skc)
`nag_1d_quad_brkpts_1` (d01slc)

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_ld_quad_gen_1(d01sjc) Example Program
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 * 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, Nag_User *comm);

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

    Vprintf("d01sjc Example Program Results\n");
    epsabs = 0.0;
    epsrel = 0.0001;
    a = 0.0;
    b = pi*2.0;
    max_num_subint = 200;
    d01sjc(f, a, b, 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\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, Nag_User *comm)
{
    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

```
d01sjc 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
```
