NAG C Library Function Document

nag_1d_quad_osc_1 (d01skc)

1 Purpose

nag_1d_quad_osc_1 (d01skc) is an adaptive integrator, especially suited to oscillating, non-singular integrands, 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_osc_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 QAG (Piessens *et al.* (1983)). It is an adaptive function, using the Gauss 30-point and Kronrod 61-point rules. A 'global' acceptance criterion (as defined by Malcolm and Simpson (1976)) is used. The local error estimation is described by Piessens *et al.* (1983).

As this function is based on integration rules of high order, it is especially suitable for non-singular oscillating integrands.

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 *Input*

On entry: the point at which the integrand f 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. 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** ≥ 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 $|I-$**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_osc_1.

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_osc_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**.

6 Further Comments

The time taken by nag_1d_quad_osc_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_osc_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, $\int_{a_i}^{b_i} f(x)dx \simeq r_i$ 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 = **sub_int_beg_pts**$[i-1]$,

b_i = **sub_int_end_pts**$[i-1]$,

r_i = **sub_int_result**$[i-1]$ and

e_i = **sub_int_error**$[i-1]$.

6.1 Accuracy

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

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

where

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

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

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

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

Piessens R (1973) An algorithm for automatic integration *Angew. Inf.* **15** 399–401

7 See Also

nag_1d_quad_gen_1 (d01sjc)
nag_1d_quad_brkpts_1 (d01slc)

8 Example

To compute

$$\int_0^{2\pi} \sin(30x) \cos x \, dx.$$

8.1 Program Text

```
/* nag_1d_quad_osc_1(d01skc) 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("d01skc Example Program Results\n");
  epsabs = 0.0;
  epsrel = 0.001;
  a = 0.0;
  b = pi * 2.0;
  max_num_subint = 200;

  d01skc(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)
{
  return x*sin(x*30.0)*cos(x);
}
```

8.2 Program Data

None.

8.3 Program Results

```
d01skc 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-03

result - approximation to the integral =  -0.20967
abserr - estimate of the absolute error =  4.49e-14
qp.fun_count  - number of function evaluations =  427
qp.num_subint  - number of subintervals used =    4
```