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).

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

f

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)
```

x

Input: the point at which the integrand f must be evaluated.

comm

Input/Output: pointer to a structure of type Nag_User with the following member:

p – Pointer

Input/Output: 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.)

a

Input: the lower limit of integration, a.

b

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

epsabs

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

epsrel
Input: the relative accuracy required. If **epsrel** is negative, the absolute value is used. See Section 6.1.

max_num_subint
Input: 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 value: a value in the range 200 to 500 is adequate for most problems.
Constraint: **max_num_subint** ≥ 1.

result
Output: the approximation to the integral I.

abserr
Output: an estimate of the modulus of the absolute error, which should be an upper bound for $|I-$**result**$|$.

qp
Pointer to structure of type Nag_QuadProgress with the following members:

num_subint – Integer
Output: the actual number of sub-intervals used.

fun_count – Integer
Output: the number of function evaluations performed by this function.

sub_int_be_pts_pts – double *
sub_int_end_pts – double *
sub_int_result – double *
sub_int_error – double *
Output: 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. If this function is to be called repeatedly, then the user should free the storage allocated by these pointers before any subsequent call is made.

comm
Input/Output: pointer to a structure of type Nag_User with the following member:

p – Pointer
Input/Output: 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 will be `void *` with a C compiler that defines `void *` and `char *` otherwise.

fail
The NAG error parameter, see the Essential Introduction to the NAG C Library.

Users are recommended to declare and initialise **fail** and set **fail.print** = TRUE for this function.

5. Error Indications 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** = $\langle$*value*$\rangle$, **epsrel** = $\langle$*value*$\rangle$.
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 ($\langle$*value*$\rangle$, $\langle$*value*$\rangle$).
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 the function 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 this function along with the integral contributions and error estimates over the sub-intervals.

Specifically, for $i = 1, 2, \ldots, n$, 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 this 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

$a_i =$ **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

De Doncker E (1978) An Adaptive Extrapolation Algorithm for Automatic Integration *ACM Signum Newsletter* **13** (2) 12–18.

Malcolm M A and Simpson R B (1976) Local Versus Global Strategies for Adaptive Quadrature *ACM Trans. Math. Softw.* **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

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

8.1. Program Text

```
/* nag_1d_quad_gen_1(d01sjc) Example Program
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 */

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

#ifdef NAG_PROTO
static double f(double x, Nag_User *comm);
#else
static double f();
#endif

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)
    {
      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);
      exit(EXIT_SUCCESS);
    }
  else
    exit(EXIT_FAILURE);
}

#ifdef NAG_PROTO
static double f(double x, Nag_User *comm)
#else
     static double f(x, comm)
     double x;
     Nag_User *comm;
#endif
{
  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
```