nag_multid_quad_adapt_1 (d01wcc)

1. Purpose

nag_multid_quad_adapt_1 (d01wcc) attempts to evaluate a multi-dimensional integral (up to 15 dimensions), with constant and finite limits,

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} \dots \int_{a_n}^{b_n} f(x_1, x_2, \dots, x_n) dx_n \dots dx_2 dx_1$$

to a specified relative accuracy, using an adaptive subdivision strategy.

2. Specification

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

3. Description

The routine evaluates an estimate of a multi-dimensional integral over a hyper-rectangle (i.e., with constant limits), and also an estimate of the relative error. The user sets the relative accuracy required, supplies the integrand as a function \mathbf{f} , and also sets the minimum and maximum acceptable number of calls to \mathbf{f} (in **minpts** and **maxpts**).

The routine operates by repeated subdivision of the hyper-rectangular region into smaller hyperrectangles. In each subregion, the integral is estimated using a seventh-degree rule, and an error estimate is obtained by comparison with a fifth-degree rule which uses a subset of the same points. The fourth differences of the integrand along each co-ordinate axis are evaluated, and the subregion is marked for possible future subdivision in half along that co-ordinate axis which has the largest absolute fourth difference.

If the estimated errors, totalled over the subregions, exceed the requested relative error (or if fewer than **minpts** calls to **f** have been made), further subdivision is necessary, and is performed on the subregion with the largest estimated error, that subregion being halved along the appropriate co-ordinate axis.

The routine will fail if the requested relative error level has not been attained by the time **maxpts** calls to \mathbf{f} have been made.

This function is based on the HALF subroutine developed by Van Dooren and De Ridder (1976). It uses a different basic rule, described by Genz and Malik (1980).

4. Parameters

ndim

Input: the number of dimensions of the integral, n. Constraint: $2 \leq \text{ndim} \leq 15$.

f

The function \mathbf{f} , supplied by the user, must return the value of the integrand f at a given point.

The specification of \mathbf{f} is:

<pre>double f(Integer ndim, double x[], Nag_User *comm)</pre>
ndim
Input: the number of dimensions of the integral.
$\mathbf{x}[\mathbf{ndim}]$
Input: the co-ordinates of the point at which the integrand 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[ndim]

Input: the lower limits of integration, a_i , for i = 1, 2, ..., n.

b[ndim]

Input: the upper limits of integration, b_i , for i = 1, 2, ..., n.

minpts

Input: **minpts** must be set to the minimum number of integrand evaluations to be allowed. Output: **minpts** contains the actual number of integrand evaluations used by this function.

maxpts

Input: the maximum number of integrand evaluations to be allowed.

Constraints: $maxpts \ge minpts$,

 $maxpts \ge 2^{ndim} + 2 \times ndim^2 + 2 \times ndim + 1.$

eps

Input: the relative error acceptable to the user. When the solution is zero or very small relative accuracy may not be achievable but the user may still set **eps** to a reasonable value and check **fail.code** for **NE_QUAD_MAX_INTEGRAND_EVAL**. Constraint: **eps** > 0.0.

finval

Output: the best estimate obtained for the integral.

acc

Output: the estimated relative error in finval.

comm

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

p - Pointer

Input/Output: the pointer \mathbf{p} , of type Pointer, allows the user to communicate information to and from the user-defined function $\mathbf{f}()$. An object of the required type should be declared by the user, e.g. a structure, and its address assigned to the pointer \mathbf{p} by means of a cast to Pointer in the calling program, e.g. comm. $\mathbf{p} = (Pointer)\&s$. 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 initialize **fail** and set **fail.print** = TRUE for this function.

5. Error Indications and Warnings

NE_INVALID_INT_RANGE_2

Value $\langle value \rangle$ given to **ndim** not valid. Correct range is $2 \leq ndim \leq 15$.

NE_2_INT_ARG_LT

On entry, $maxpts = \langle value \rangle$ while $minpts = \langle value \rangle$. These parameters must satisfy $maxpts \ge minpts$.

NE_QUAD_MAX_INTEGRAND_CONS

maxpts $\langle value \rangle$. Constraint: maxpts $\geq 2^{ndim} + 2 \times ndim^2 + 2 \times ndim + 1$.

NE_REAL_ARG_LE

On entry, **eps** must not be less than or equal to 0.0: **eps** = $\langle value \rangle$.

NE_ALLOC_FAIL

Memory allocation failed.

NE_QUAD_MAX_INTEGRAND_EVAL

maxpts was too small to obtain the required accuracy.

On return, **finval** and **acc** contain estimates of the integral and the relative error, but **acc** will be greater than **eps**.

6. Further Comments

Execution time will usually be dominated by the time taken to evaluate the integrand \mathbf{f} , and hence the maximum time that could be taken will be proportional to **maxpts**.

6.1. Accuracy

A relative error estimate is output through the parameter acc.

6.2. References

Genz A C and Malik A A (1980) An Adaptive Algorithm for Numerical Integration over an Ndimensional Rectangular Region J. Comput. Appl. Math. 6 295–302.

Van Dooren P and De Ridder L (1976) An Adaptive Algorithm for Numerical Integration over an N-dimensional Cube J. Comput. Appl. Math. 2 (3) 207–217.

7. See Also

nag_multid_quad_monte_carlo_1 (d01xbc)

8. Example

This example program estimates the integral

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{4z_1 z_3^2 \exp(2z_1 z_3)}{(1+z_2+z_4)^2} dz_4 dz_3 dz_2 dz_1 = 0.575364.$$

The accuracy requested is one part in 10,000.

8.1. Program Text

```
/* nag_multid_quad_adapt_1(d01wcc) Example Program
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 */
#include <nag.h>
#include <stdio.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagd01.h>
#ifdef NAG_PROTO
static double f(Integer n, double z[], Nag_User *comm);
#else
static double f();
#endif
```

```
#define NDIM 4
     #define MAXPTS 1000*NDIM
     main()
     {
       Integer ndim = NDIM;
       Integer maxpts = MAXPTS;
       double a[4], b[4];
       Integer k;
       static NagError fail;
       double finval;
       Integer minpts;
       double acc, eps;
       Nag_User comm;
       Vprintf("d01wcc Example Program Results\n");
       for (k=0; k < 4; ++k)
         {
           a[k] = 0.0;
           b[k] = 1.0;
         }
       eps = 0.0001;
       minpts = 0;
       d01wcc(ndim, f, a, b, &minpts, maxpts, eps, &finval, &acc, &comm, &fail);
       if (fail.code != NE_NOERROR)
         Vprintf("%s\n",fail.message);
       if (fail.code == NE_NOERROR || fail.code == NE_QUAD_MAX_INTEGRAND_EVAL)
         {
           Vprintf("Requested accuracy =%12.2e\n", eps);
Vprintf("Estimated value =%12.4f\n", finval);
           Vprintf("Estimated accuracy =%12.2e\n", acc);
           exit(EXIT_SUCCESS);
         }
       else
         exit(EXIT_FAILURE);
     }
     #ifdef NAG_PROTO
     static double f(Integer n, double z[], Nag_User *comm)
     #else
          static double f(n, z, comm)
          Integer n;
          double z[];
          Nag_User *comm;
     #endif
     ſ
       double tmp_pwr;
       tmp_pwr = z[1]+1.0+z[3];
       return z[0]*4.0*z[2]*z[2]*exp(z[0]*2.0*z[2])/(tmp_pwr*tmp_pwr);
     7
8.2. Program Data
     None.
8.3. Program Results
     d01wcc Example Program Results
    Requested accuracy = 1.00e-04
Estimated value = 0.5754
     Estimated accuracy =
                            9.89e-05
```