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nag_multid_quad_adapt (d01fcc)

1. Purpose

nag_multid_quad_adapt (d01fcc) 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

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 hyper-rectangles. 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 \mathbf{maxpts} calls to \mathbf{f} have been made.

nag_multid_quad_adapt 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: $2 \le \text{ndim} \le 15$.

 \mathbf{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:

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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 $i=1,2,\ldots,n$.

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 the function nag_multid_quad_adapt.

maxpts

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

Constraints: $maxpts \ge minpts$.

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

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**.

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 $2 \leq \text{ndim} \leq 15$.

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

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

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

 \mathbf{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.

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6.2. References

Genz A C and Malik A A (1980) An Adaptive Algorithm for Numerical Integration over an N-dimensional 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 (d01gbc)

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(d01fcc) Example Program
 * Copyright 1991 Numerical Algorithms Group.
 * Mark 2, 1991.
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagd01.h>
#ifdef NAG_PROTO
static double f(Integer n, double z[]);
#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;
  Vprintf("d01fcc Example Program Results\n");
  for (k=0; k < 4; ++k)
      a[k] = 0.0;
      b[k] = 1.0;
  eps = 0.0001;
  minpts = 0;
  d01fcc(ndim, f, a, b, &minpts, maxpts, eps, &finval, &acc, &fail);
  if (fail.code != NE_NOERROR)
    Vprintf("%s\n",fail.message);
  if (fail.code == NE_NOERROR | | fail.code == NE_QUAD_MAX_INTEGRAND_EVAL)
```

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```
{
    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[])
#else
    static double f(n, z)
    Integer n;
    double z[];
#endif
{
    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);
}
```

8.2. Program Data

None.

8.3. Program Results

d01fcc Example Program Results
Requested accuracy = 1.00e-04
Estimated value = 0.5754
Estimated accuracy = 9.89e-05

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