NAG Library Function Document

nag_multid_quad_adapt_1 (d01wcc)

1 Purpose

nag_multid_quad_adapt_1 (d01wcc) attempts to evaluate a multidimensional integral (up to 15 dimensions), with constant and finite limits,
\[ \int_{a_1}^{b_1} \int_{a_2}^{b_2} \cdots \int_{a_n}^{b_n} f(x_1, x_2, \ldots, x_n) \, dx_n \cdots dx_2 dx_1 \]
to a specified relative accuracy, using an adaptive subdivision strategy.

2 Specification

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

void nag_multid_quad_adapt_1 (Integer ndim,
   double (*f)(Integer ndim, const double x[], Nag_User *comm),
   const double a[], const double b[], Integer *minpts, Integer maxpts,
   double eps, double *finval, double *acc, Nag_User *comm, NagError *fail)
```

3 Description

nag_multid_quad_adapt_1 (d01wcc) evaluates an estimate of a multidimensional integral over a hyper-rectangle (i.e., with constant limits), and also an estimate of the relative error. You will need to set the relative accuracy required, supply the integrand as a function \( f \), and also set the minimum and maximum acceptable number of calls to \( f \) (in \texttt{minpts} and \texttt{maxpts}).

The function 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 coordinate axis are evaluated, and the subregion is marked for possible future subdivision in half along that coordinate 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 \texttt{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 coordinate axis.

The function will fail if the requested relative error level has not been attained by the time \texttt{maxpts} calls to \( f \) 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 References


5 Arguments

1: \texttt{ndim} – Integer \hspace{1cm} \textit{Input}

\textit{On entry:} the number of dimensions of the integral, \( n \).
\textit{Constraint:} \( 2 \leq \texttt{ndim} \leq 15 \).

2: \texttt{f} – function, supplied by the user \hspace{1cm} \textit{External Function}

\texttt{f} must return the value of the integrand \( f \) at a given point.

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The specification of \texttt{f} is:
\[
\text{double f (Integer ndim, const double x[], Nag_User *comm)}
\]

1: \texttt{ndim} – Integer \hspace{1cm} \textit{Input}

\textit{On entry:} the number of dimensions of the integral.

2: \texttt{x[ndim]} – const double \hspace{1cm} \textit{Input}

\textit{On entry:} the coordinates of the point at which the integrand must be evaluated.

3: \texttt{comm} – Nag_User *

Pointer to a structure of type Nag_User with the following member:

\texttt{p} – Pointer

\textit{On entry/exit:} the pointer \texttt{comm->p} should be cast to the required type, e.g.,
\[
\text{struct user *} s = (\text{struct user *} \text{comm}) \to p,
\]

\texttt{p} to obtain the original object's address with appropriate type. (See the argument \texttt{comm} below.)

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3: \texttt{a[ndim]} – const double \hspace{1cm} \textit{Input}

\textit{On entry:} the lower limits of integration, \( a_i \), for \( i = 1, 2, \ldots, n \).

4: \texttt{b[ndim]} – const double \hspace{1cm} \textit{Input}

\textit{On entry:} the upper limits of integration, \( b_i \), for \( i = 1, 2, \ldots, n \).

5: \texttt{minpts} – Integer * \hspace{1cm} \textit{Input/Output}

\textit{On entry:} \texttt{minpts} must be set to the minimum number of integrand evaluations to be allowed.
\textit{On exit:} \texttt{minpts} contains the actual number of integrand evaluations used by this function.

6: \texttt{maxpts} – Integer \hspace{1cm} \textit{Input}

\textit{On entry:} the maximum number of integrand evaluations to be allowed.
\textit{Constraints:}
\[
\text{maxpts} \geq \text{minpts}; \\
\text{maxpts} \geq 2^{\text{ndim}} + 2 \times \text{ndim}^2 + 2 \times \text{ndim} + 1.
\]

7: \texttt{eps} – double \hspace{1cm} \textit{Input}

\textit{On entry:} the relative error acceptable. When the solution is zero or very small relative accuracy may not be achievable but you may still set \texttt{eps} to a reasonable value and check \texttt{fail} for NE_QUAD_MAX_INTEGRAND_EVAL.
\textit{Constraint:} \texttt{eps} > 0.0.
8: \texttt{finval} – double *  
\textit{Output} \quad On exit: the best estimate obtained for the integral.

9: \texttt{acc} – double *  
\textit{Output} \quad On exit: the estimated relative error in \texttt{finval}.

10: \texttt{comm} – Nag_User *  
Pointer to a structure of type Nag_User with the following member:

\begin{itemize}
  \item \texttt{p} – Pointer \quad \textit{On entry/exit}: the pointer \texttt{comm->p}, of type Pointer, allows you to communicate information to and from \texttt{f()}. An object of the required type should be declared, e.g., a structure, and its address assigned to the pointer \texttt{comm->p} by means of a cast to Pointer in the calling program, e.g., \texttt{comm.p = (Pointer)&s}. The type pointer will be \texttt{void *} with a C compiler that defines \texttt{void *} and \texttt{char *} otherwise.
\end{itemize}

11: \texttt{fail} – NagError *  
\textit{Input/Output} \quad The NAG error argument (see Section 3.6 in the Essential Introduction).

6 \quad \textbf{Error Indicators and Warnings}

\textbf{NE_2_INT_ARG_LT}  
On entry, \texttt{maxpts} = \langle value \rangle while \texttt{minpts} = \langle value \rangle. These arguments must satisfy \texttt{maxpts} \geq \texttt{minpts}.

\textbf{NE_ALLOC_FAIL}  
Dynamic memory allocation failed.

\textbf{NE_INVALID_INT_RANGE_2}  
Value \langle value \rangle given to \texttt{ndim} not valid. Correct range is 2 \leq \texttt{ndim} \leq 15.

\textbf{NE_QUAD_MAX_INTEGRAND_CONS}  
\texttt{maxpts} < \langle value \rangle. Constraint: \texttt{maxpts} \geq 2^{\texttt{ndim}} + 2 \times \texttt{ndim}^2 + 2 \times \texttt{ndim} + 1.

\textbf{NE_QUAD_MAX_INTEGRAND_EVAL}  
\texttt{maxpts} was too small to obtain the required accuracy. On return, \texttt{finval} and \texttt{acc} contain estimates of the integral and the relative error, but \texttt{acc} will be greater than \texttt{eps}.

\textbf{NE_REAL_ARG_LE}  
On entry, \texttt{eps} must not be less than or equal to 0.0: \texttt{eps} = \langle value \rangle.

7 \quad \textbf{Accuracy}

A relative error estimate is output through the argument \texttt{acc}.

8 \quad \textbf{Parallelism and Performance}

Not applicable.
9 Further Comments

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

10 Example

This example estimates the integral

$$
\int_0^1 \int_0^1 \int_0^1 \int_0^1 4z_1z_2^2 \exp(2z_1z_3) \frac{dz_4}{(1+z_2+z_4)^2}dz_3dz_2dz_1 = 0.575364.
$$

The accuracy requested is one part in 10,000.

10.1 Program Text

```c
/* nag_multid_quad_adapt_1 (d01wcc) Example Program. */
/* Copyright 2014 Numerical Algorithms Group. */
/* Mark 5, 1998. */
/* Mark 7 revised, 2001. */
*/
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagd01.h>

#ifdef __cplusplus
extern "C" {
#endif
static double NAG_CALL f(Integer n, const double z[], Nag_User *comm);
#ifdef __cplusplus
}
#endif
#define NDIM 4
#define MAXPTS 1000*NDIM

int main(void)
{
    static Integer use_comm[1] = {1};
    Integer exit_status = 0;
    Integer ndim = NDIM;
    Integer maxpts = MAXPTS;
    double a[4], b[4];
    Integer k;
    double finval;
    Integer minpts;
    double acc, eps;
    Nag_User comm;
    NagError fail;

    INIT_FAIL(fail);

    printf("nag_multid_quad_adapt_1 (d01wcc) Example Program Results\n");
    /* For communication with user-supplied functions: */
    comm.p = (Pointer)&use_comm;

    for (k = 0; k < 4; ++k)
    {
        a[k] = 0.0;
        b[k] = 1.0;
    }
    d01wcc
```
eps = 0.0001;
minpts = 0;

/* nag_multid_quad_adapt_1 (d01wcc).
 * Multi-dimensional adaptive quadrature, thread-safe
 */
nag_multid_quad_adapt_1(ndim, f, a, b, &minpts, maxpts, eps, &finval, &acc, 
&comm, &fail);

if (fail.code != NE_NOERROR && fail.code != NE_QUAD_MAX_INTEGRAND_EVAL)
{
    printf("Error from nag_multid_quad_adapt_1 (d01wcc) %s\n", 
    fail.message);
    exit_status = 1;
    goto END;
}
printf("Requested accuracy =%12.2e\n", eps);
printf("Estimated value =%12.4f\n", finval);
printf("Estimated accuracy =%12.2e\n", acc);

END:
return exit_status;
}

static double NAG_CALL f(Integer n, const double z[], Nag_User *comm)
{
    double tmp_pwr;
    Integer *use_comm = (Integer *)comm->p;

    if (use_comm[0])
    {
        printf("(User-supplied callback f, first invocation.)\n");
        use_comm[0] = 0;
    }
    tmp_pwr = z[1]+1.0+z[n-1];
    return z[0]*4.0*z[2]*z[2]*exp(z[0]*2.0*z[2])/(tmp_pwr*tmp_pwr);
}

10.2 Program Data
None.

10.3 Program Results
nag_multid_quad_adapt_1 (d01wcc) Example Program Results
(User-supplied callback f, first invocation.)
Requested accuracy = 1.00e-04
Estimated value = 0.5754
Estimated accuracy = 9.89e-05