NAG C Library Function Document

nag_1d_quad_osc (d01akc)

1 Purpose

nag_1d_quad_osc (d01akc) 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 (double (*f)(double),
    double a, double b, double epsabs, double epsrel,
    Integer max_num_subint, double *result, double *abserr,
    Nag_QuadProgress *qp, 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

\( \text{Function} \)

The function \( f \), supplied by the user, must return the value of the integrand \( f \) at a given point.

The specification of \( f \) is:

\[
\text{double } f(\text{double } x)
\]

1: \( x \) – double

\( \text{Input} \)

\( \text{On entry:} \) the point at which the integrand \( f \) must be evaluated.

2: \( a \) – double

\( \text{Input} \)

\( \text{On entry:} \) the lower limit of integration, \( a \).

3: \( b \) – double

\( \text{Input} \)

\( \text{On entry:} \) the upper limit of integration, \( b \). It is not necessary that \( a < b \).

4: \( \text{epsabs} \) – double

\( \text{Input} \)

\( \text{On entry:} \) the absolute accuracy required. If \( \text{epsabs} \) is negative, the absolute value is used. See Section 6.1.

[NP3491/6]
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.

   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 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: 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: \texttt{max\_num\_subint} = \texttt{<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 \texttt{epsabs} and \texttt{epsrel}, or increasing the value of
\texttt{max\_num\_subint}.

NE_QUAD_ROUNDOFF_TOL

Round-off error prevents the requested tolerance from being achieved: \texttt{epsabs} = \texttt{<value>},
\texttt{epsrel} = \texttt{<value>},

The error may be underestimated. Consider relaxing the accuracy requirements specified by \texttt{epsabs}
and \texttt{epsrel}.

NE_QUAD_BAD_SUBDIV

Extremely bad integrand behaviour occurs around the sub-interval \texttt{(<value>, <value>)},
The same advice applies as in the case of \texttt{NE_QUAD_MAX_SUBDIV}.

6 Further Comments

The time taken by nag_1d_quad_osc depends on the integrand and the accuracy required.

If the function fails with an error exit other than \texttt{NE_INT_ARG_LT} or \texttt{NE_ALLOC_FAIL}, then the user
may wish to examine the contents of the structure \texttt{qp}. These contain the end-points of the sub-intervals
used by nag_1d_quad_osc along with the integral contributions and error estimates over these 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, \( \int_{a_i}^{b_i} f(x) \, dx \approx r_i \) and \( \texttt{result} = \sum_{i=1}^{n} r_i \). The value of \( n \) is returned in \texttt{num\_subint}, and the values \( a_i, b_i, r_i \) and \( e_i \) are stored in the structure \texttt{qp} as

\[
\begin{align*}
a_i &= \texttt{sub\_int\_beg\_pts}[i-1], \\
b_i &= \texttt{sub\_int\_end\_pts}[i-1], \\
r_i &= \texttt{sub\_int\_result}[i-1] \quad \text{and} \\
e_i &= \texttt{sub\_int\_error}[i-1].
\end{align*}
\]

6.1 Accuracy

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

\[ |I - \texttt{result}| \leq \texttt{tol} \]

where

\[ \texttt{tol} = \max\{|\texttt{epsabs}|, |\texttt{epsrel}| \times |I|\} \]

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

\[ |I - \texttt{result}| \leq \texttt{abserr} \leq \texttt{tol}. \]

6.2 References


\[\text{[NP3491/6]}\]
7 See Also

nag_1d_quad_gen (d01ajc)
nag_1d_quad_brkpts (d01alc)

8 Example

To compute

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

8.1 Program Text

/* nag_1d_quad_oscr (d01akc) Example Program */

* * Mark 2, 1991.
* * 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);

main()
{
    double a, b;
    double epsabs, abseps, epsrel, result;
    Nag_QuadProgress qp;
    Integer max_num_subint;
    static NagError fail;
    double pi = X01AAC;

    Vprintf("d01akc Example Program Results\n");
    epsabs = 0.0;
    epsrel = 0.001;
    a = 0.0;
    b = pi * 2.0;
    max_num_subint = 200;

    d01akc(f, a, b, epsabs, abseps, epsrel, max_num_subint, &result, &abseps, &epsrel, &qp, &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", 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)
{
    return x*sin(x*30.0)*cos(x);
}

8.2 Program Data
None.

8.3 Program Results

d01akc 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