

NAG C Library Function Document

nag_1d_quad_wt_trig_1 (d01snc)

1 Purpose

nag_1d_quad_wt_trig_1 (d01snc) calculates an approximation to the sine or the cosine transform of a function g over $[a, b]$:

$$I = \int_a^b g(x) \sin(\omega x) dx \quad \text{or} \quad I = \int_a^b g(x) \cos(\omega x) dx$$

(for a user-specified value of ω).

2 Specification

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

void nag_1d_quad_wt_trig_1 (double (*g)(double x, Nag_User *comm),
    double a, double b, double omega, Nag_TrigTransform wt_func,
    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 QFOUR (Piessens *et al.* (1983)). It is an adaptive routine, designed to integrate a function of the form $g(x)w(x)$, where $w(x)$ is either $\sin(\omega x)$ or $\cos(\omega x)$. If a sub-interval has length

$$L = |b - a|2^{-l}$$

then the integration over this sub-interval is performed by means of a modified Clenshaw-Curtis procedure (Piessens and Branders (1975)) if $L\omega > 4$ and $l \leq 20$. In this case a Chebyshev-series approximation of degree 24 is used to approximate $g(x)$, while an error estimate is computed from this approximation together with that obtained using Chebyshev-series of degree 12. If the above conditions do not hold then Gauss 7-point and Kronrod 15-point rules are used. The algorithm, described in Piessens *et al.* (1983), incorporates a global acceptance criterion (as defined in Malcolm and Simpson (1976)) together with the ϵ -algorithm (Wynn (1956)) to perform extrapolation. The local error estimation is described in Piessens *et al.* (1983).

4 Parameters

1: **g** – function supplied by user *Function*

The function **g**, supplied by the user, must return the value of the function g at a given point.

The specification of **g** is:

```
double g(double x, Nag_User *comm)
```

1: **x** – double *Input*

On entry: the point at which the function g must be evaluated.

- | | | |
|----|---|--|
| 2: | <p>comm – Nag_User *</p> <p><i>On entry/on exit:</i> pointer to a structure of type Nag_User with the following member:</p> <p style="text-align: center;">p – Pointer <i>Input/Output</i></p> <p><i>On entry/on exit:</i> the pointer comm→p should be cast to the required type, e.g.,
 <code>struct user *s = (struct user *)comm->p</code>, to obtain the original object's address with appropriate type. (See the argument comm below.)</p> | |
|----|---|--|
-
- | | | |
|-----|--|--|
| 2: | <p>a – double <i>Input</i></p> <p><i>On entry:</i> the lower limit of integration, <i>a</i>.</p> | |
| 3: | <p>b – double <i>Input</i></p> <p><i>On entry:</i> the upper limit of integration, <i>b</i>. It is not necessary that $a < b$.</p> | |
| 4: | <p>omega – double <i>Input</i></p> <p><i>On entry:</i> the parameter ω in the weight function of the transform.</p> | |
| 5: | <p>wt_func – Nag_TrigTransform <i>Input</i></p> <p><i>On entry:</i> indicates which integral is to be computed:</p> <p style="padding-left: 20px;">if wt_func = Nag_Cosine, $w(x) = \cos(\omega x)$;</p> <p style="padding-left: 20px;">if wt_func = Nag_Sine, $w(x) = \sin(\omega x)$.</p> <p><i>Constraint:</i> wt_func = Nag_Cosine or Nag_Sine.</p> | |
| 6: | <p>epsabs – double <i>Input</i></p> <p><i>On entry:</i> the absolute accuracy required. If epsabs is negative, the absolute value is used. See Section 6.1.</p> | |
| 7: | <p>epsrel – double <i>Input</i></p> <p><i>On entry:</i> the relative accuracy required. If epsrel is negative, the absolute value is used. See Section 6.1.</p> | |
| 8: | <p>max_num_subint – Integer <i>Input</i></p> <p><i>On entry:</i> 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.</p> <p><i>Suggested values:</i> a value in the range 200 to 500 is adequate for most problems.</p> <p><i>Constraint:</i> max_num_subint ≥ 1.</p> | |
| 9: | <p>result – double * <i>Output</i></p> <p><i>On exit:</i> the approximation to the integral <i>I</i>.</p> | |
| 10: | <p>abserr – double * <i>Output</i></p> <p><i>On exit:</i> an estimate of the modulus of the absolute error, which should be an upper bound for $I - \mathbf{result}$.</p> | |

11: **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_wt_trig_1.

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**, **NE_BAD_PARAM** 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_wt_trig_1 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**.

12: **comm** – Nag_User *

On entry/on exit: pointer to a structure of type **Nag_User** with the following member:

p – Pointer *Input/Output*

On entry/on exit: the pointer **p**, of type Pointer, allows the user to communicate information to and from the user-defined function **g()**. 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 is `void *`.

13: **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_BAD_PARAM

On entry, parameter **wt_func** had an illegal 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** = *<value>*, **epsrel** = *<value>*.

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 (*<value>*, *<value>*).

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 also occur with any error exit other than **NE_INT_ARG_LT**, **NE_BAD_PARAM** or **NE_ALLOC_FAIL**.

6 Further Comments

The time taken by `tnag_1d_quad_wt_trig_1` depends on the integrand and the accuracy required.

If the function fails with an error exit other than **NE_INT_ARG_LT**, **NE_BAD_PARAM** 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 `nag_1d_quad_wt_trig_1` along with the integral contributions and error estimates over the sub-intervals.

Specifically, for $i = 1, 2, \dots, n$, 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, $\int_{a_i}^{b_i} g(x)w(x) dx \simeq r_i$ and **result** = $\sum_{i=1}^n r_i$ unless the 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

$$a_i = \text{sub_int_beg_pts}[i - 1],$$

$$b_i = \text{sub_int_end_pts}[i - 1],$$

$$r_i = \text{sub_int_result}[i - 1] \text{ and}$$

$$e_i = \text{sub_int_error}[i - 1].$$

6.1 Accuracy

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

$$|I - \text{result}| \leq \text{tol}$$

where

$$\text{tol} = \max\{|\text{epsabs}|, |\text{epsrel}| \times |I|\}$$

and **epsabs** and **epsrel** are user-specified absolute and relative error tolerances. Moreover it returns the

quantity **abserr** which, in normal circumstances, satisfies

$$|I - \text{result}| \leq \text{abserr} \leq \text{tol}.$$

6.2 References

Malcolm M A and Simpson R B (1976) Local versus global strategies for adaptive quadrature *ACM Trans. Math. Software* **1** 129–146

Piessens R and Branders M (1975) Algorithm 002. Computation of oscillating integrals *J. Comput. Appl. Math.* **1** 153–164

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_gen_1 (d01sjc)

8 Example

To compute

$$\int_0^1 \ln x \sin(10\pi x) dx.$$

8.1 Program Text

```
/* nag_1d_quad_wt_trig_1(d01snc) Example Program
 *
 * Copyright 1998 Numerical Algorithms Group.
 *
 * Mark 5, 1998.
 *
 * 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 g(double x, Nag_User *comm);

main()
{
    double a, b;
    double omega;
    double epsabs, abserr, epsrel, result;
    Nag_TrigTransform wt_func;
    Nag_QuadProgress qp;
    Integer max_num_subint;
    static NagError fail;
    Nag_User comm;
```

```

Vprintf("d01snc Example Program Results\n");
epsrel = 0.0001;
epsabs = 0.0;
a = 0.0;
b = 1.0;
omega = X01AAC * 10.0;
wt_func = Nag_Sine;
max_num_subint = 200;
d01snc(g, a, b, omega, wt_func, 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 && fail.code != NE_BAD_PARAM &&
    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);
  }
exit(EXIT_FAILURE);
}

static double g(double x, Nag_User *comm)
{
  return (x>0.0) ? log(x) : 0.0;
}

```

8.2 Program Data

None.

8.3 Program Results

```

d01snc Example Program Results
a      - lower limit of integration =      0.0000
b      - upper limit of integration =      1.0000
epsabs - absolute accuracy requested = 0.00e+00
epsrel - relative accuracy requested = 1.00e-04

result - approximation to the integral = -0.12814
abserr - estimate of the absolute error = 3.58e-06
qp.fun_count - number of function evaluations = 275
qp.num_subint - number of subintervals used =      8

```