NAG Toolbox

nag_quad_1d_fin_wcauchy (d01aq)

1 Purpose

nag_quad_1d_fin_wcauchy (d01aq) calculates an approximation to the Hilbert transform of a function $g(x)$ over $[a, b]$:

$$I = \int_a^b \frac{g(x)}{x - c} dx$$

for user-specified values of a, b and c.

2 Syntax

```
[result, abserr, w, iw, ifail] = nag_quad_1d_fin_wcauchy(g, a, b, c, epsabs,
epsrel, 'lw', lw, 'liw', liw)
```

```
[result, abserr, w, iw, ifail] = d01aq(g, a, b, c, epsabs, epsrel, 'lw', lw,
'liw', liw)
```

3 Description

nag_quad_1d_fin_wcauchy (d01aq) is based on the QUADPACK routine QAWC (see Piessens *et al.* (1983)) and integrates a function of the form $g(x)w(x)$, where the weight function

$$w(x) = \frac{1}{x - c}$$

is that of the Hilbert transform. (If $a < c < b$ the integral has to be interpreted in the sense of a Cauchy principal value.) It is an adaptive function which employs a ‘global’ acceptance criterion (as defined by Malcolm and Simpson (1976)). Special care is taken to ensure that c is never the end point of a sub-interval (see Piessens *et al.* (1976)). On each sub-interval (c_1, c_2) modified Clenshaw–Curtis integration of orders 12 and 24 is performed if $c_1 - d \leq c \leq c_2 + d$ where $d = (c_2 - c_1)/20$. Otherwise the Gauss 7-point and Kronrod 15-point rules are used. The local error estimation is described by Piessens *et al.* (1983).

4 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, de Doncker–Kapenga E, Ûberhuber C and Kahaner D (1983) *QUADPACK, A Subroutine Package for Automatic Integration* Springer–Verlag

Piessens R, van Roy–Branders M and Mertens I (1976) The automatic evaluation of Cauchy principal value integrals *Angew. Inf.* **18** 31–35

5 Parameters

5.1 Compulsory Input Parameters

1: **g** – REAL (KIND=nag_wp) FUNCTION, supplied by the user.

g must return the value of the function g at a given point **x**.

```
[result] = g(x)
```

Input Parameters

1: **x** – REAL (KIND=nag_wp)

The point at which the function g must be evaluated.

Output Parameters

1: **result**

The value of $g(x)$ evaluated at **x**.

2: **a** – REAL (KIND=nag_wp)

a, the lower limit of integration.

3: **b** – REAL (KIND=nag_wp)

b, the upper limit of integration. It is not necessary that $a < b$.

4: **c** – REAL (KIND=nag_wp)

The argument c in the weight function.

Constraint: **c** must not equal **a** or **b**.

5: **epsabs** – REAL (KIND=nag_wp)

The absolute accuracy required. If **epsabs** is negative, the absolute value is used. See Section 7.

6: **epsrel** – REAL (KIND=nag_wp)

The relative accuracy required. If **epsrel** is negative, the absolute value is used. See Section 7.

5.2 Optional Input Parameters

1: **lw** – INTEGER

Suggested value: **lw** $= 800$ to 2000 is adequate for most problems.

Default: 800

The dimension of the array **w**. the value of **lw** (together with that of **liw**) imposes a bound on the number of sub-intervals into which the interval of integration may be divided by the function. The number of sub-intervals cannot exceed **lw**$/4$. The more difficult the integrand, the larger **lw** should be.

Constraint: **lw** ≥ 4.

2: **liw** – INTEGER

Suggested value: **liw** $=$ **lw**$/4$.

Default: **lw**$/4$

The dimension of the array **iw**. the number of sub-intervals into which the interval of integration may be divided cannot exceed **liw**.

Constraint: **liw** ≥ 1.

5.3 Output Parameters

1: **result** – REAL (KIND=nag_wp)

The approximation to the integral I.

2: **abserr** – REAL (KIND=nag_wp)

An estimate of the modulus of the absolute error, which should be an upper bound for $|I - \textbf{result}|$.

3: **w**(**lw**) – REAL (KIND=nag_wp) array

Details of the computation see Section 9 for more information.

4: **iw**(**liw**) – INTEGER array

iw(1) contains the actual number of sub-intervals used. The rest of the array is used as workspace.

5: **ifail** – INTEGER

ifail $= 0$ unless the function detects an error (see Section 5).

6 Error Indicators and Warnings

Note: nag_quad_1d_fin_wcauchy (d01aq) may return useful information for one or more of the following detected errors or warnings.

Errors or warnings detected by the function:

ifail $= 1$ (*warning*)

The maximum number of subdivisions allowed with the given workspace has been reached without the accuracy requirements being achieved. Look at the integrand in order to determine the integration difficulties. 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 amount of workspace.

ifail $= 2$ (*warning*)

Round-off error prevents the requested tolerance from being achieved. Consider requesting less accuracy.

ifail $= 3$ (*warning*)

Extremely bad local behaviour of $g(x)$ causes a very strong subdivision around one (or more) points of the interval. The same advice applies as in the case of **ifail** $= 1$.

ifail $= 4$

On entry, **c** $=$ **a** or **c** $=$ **b**.

ifail $= 5$

On entry, **lw** < 4,
or **liw** < 1.

ifail $= -99$

An unexpected error has been triggered by this routine. Please contact NAG.

ifail $= -399$

Your licence key may have expired or may not have been installed correctly.

ifail $= -999$

Dynamic memory allocation failed.

7 Accuracy

nag_quad_1d_fin_wcauchy (d01aq) cannot guarantee, but in practice usually achieves, the following accuracy:

$$|I - \textbf{result}| \leq tol,$$

where

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

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

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

8 Further Comments

The time taken by nag_quad_1d_fin_wcauchy (d01aq) depends on the integrand and the accuracy required.

If **ifail** $\neq 0$ on exit, then you may wish to examine the contents of the array **w**, which contains the end points of the sub-intervals used by nag_quad_1d_fin_wcauchy (d01aq) 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, $\int_{a_i}^{b_i} g(x)w(x)\,dx \simeq r_i$ and $\textbf{result} = \sum_{i=1}^{n} r_i$. The value of n is returned in $\textbf{iw}(1)$, and the values a_i, b_i, e_i and r_i are stored consecutively in the array **w**, that is:

$a_i = \textbf{w}(i)$,

$b_i = \textbf{w}(n + i)$,

$e_i = \textbf{w}(2n + i)$ and

$r_i = \textbf{w}(3n + i)$.

9 Example

This example computes the Cauchy principal value of

$$\int_{-1}^{1} \frac{dx}{\left(x^2 + 0.01^2\right)\left(x - \frac{1}{2}\right)}.$$

9.1 Program Text

```
function d01aq_example

fprintf('d01aq example results\n\n');

a = -1;
b = 1;
c = 0.5;
epsabs = 0;
epsrel = 0.0001;
[result, abserr, w, iw, ifail] = d01aq(@g, a, b, c, epsabs, epsrel);
```

```
fprintf('Result = %13.2f,  Standard error = %10.2e\n', result, abserr);

function result = g(x)
  result = 1/(x^2+0.01^2);
```

9.2 Program Results

```
     d01aq example results

Result =       -628.46,  Standard error =   1.32e-02
```