D01 – Quadrature d01ga

# **NAG Toolbox for MATLAB**

# d01ga

# 1 Purpose

d01ga integrates a function which is specified numerically at four or more points, over the whole of its specified range, using third-order finite-difference formulae with error estimates, according to a method due to

Gill and Miller.

# 2 Syntax

[ans, er, ifail] = 
$$d01ga(x, y, 'n', n)$$

## 3 Description

d01ga evaluates the definite integral

$$I = \int_{x_n}^{x_n} y(x) \, dx,$$

where the function y is specified at the n-points  $x_1, x_2, \ldots, x_n$ , which should be all distinct, and in either ascending or descending order. The integral between successive points is calculated by a four-point finite-difference formula centred on the interval concerned, except in the case of the first and last intervals, where four-point forward and backward difference formulae respectively are employed. If n is less than 4, the function fails. An approximation to the truncation error is integrated and added to the result. It is also returned separately to give an estimate of the uncertainty in the result. The method is due to Gill and Miller 1972.

## 4 References

Gill P E and Miller G F 1972 An algorithm for the integration of unequally spaced data *Comput. J.* 15 80–83

## 5 Parameters

### 5.1 Compulsory Input Parameters

1:  $\mathbf{x}(\mathbf{n})$  – double array

The values of the independent variable, i.e., the  $x_1, x_2, \dots, x_n$ .

Constraint: either  $\mathbf{x}(1) < \mathbf{x}(2) < \cdots < \mathbf{x}(\mathbf{n})$  or  $\mathbf{x}(1) > \mathbf{x}(2) > \cdots > \mathbf{x}(\mathbf{n})$ .

2: y(n) – double array

The values of the dependent variable  $y_i$  at the points  $x_i$ , for i = 1, 2, ..., n.

# 5.2 Optional Input Parameters

1:  $n - int32 \ scalar$ 

*Default*: The dimension of the arrays  $\mathbf{x}$ ,  $\mathbf{y}$ . (An error is raised if these dimensions are not equal.) n, the number of points.

Constraint:  $\mathbf{n} \geq 4$ .

[NP3663/21] d01ga.1

d01ga NAG Toolbox Manual

### 5.3 Input Parameters Omitted from the MATLAB Interface

None.

### 5.4 Output Parameters

#### 1: ans – double scalar

The estimated value of the integral.

#### 2: **er – double scalar**

An estimate of the uncertainty in ans.

#### 3: ifail – int32 scalar

0 unless the function detects an error (see Section 6).

# 6 Error Indicators and Warnings

Errors or warnings detected by the function:

#### ifail = 1

Indicates that fewer than four points have been supplied to d01ga.

#### ifail = 2

Values of x are neither strictly increasing nor strictly decreasing.

#### ifail = 3

Two points have the same X-value.

No error is reported arising from the relative magnitudes of ans and er on return, due to the difficulty when the true answer is zero.

### 7 Accuracy

No accuracy level is specified by you before calling d01ga but on return the absolute value of **er** is an approximation to, but not necessarily a bound for,  $|I - \mathbf{ans}|$ . If on exit **ifail** > 0, both **ans** and **er** are returned as zero.

### **8** Further Comments

The time taken by d01ga depends on the number of points supplied, n.

In their paper, Gill and Miller 1972 do not add the quantity **er** to **ans** before return. However, extensive tests have shown that a dramatic reduction in the error often results from such addition. In other cases, it does not make an improvement, but these tend to be cases of low accuracy in which the modified answer is not significantly inferior to the unmodified one. You have the option of recovering the Gill–Miller answer by subtracting **er** from **ans** on return from the function.

## 9 Example

```
x = [0;

0.04;

0.08;

0.12;

0.22;

0.26;
```

d01ga.2 [NP3663/21]

D01 – Quadrature d01ga

```
0.3;
0.38;
     0.39;
     0.42;
     0.45;
     0.46;
     0.6;
     0.68;
     0.72;
     0.73;
     0.83;
     0.85;
     0.88;
     0.9;
     1];
y = [4; 3.9936;
     3.9746;
     3.9432;
     3.8153;
     3.7467;
     3.6697;
     3.4943;
     3.4719;
     3.4002;
     3.3264;
     3.3014;
     2.9412;
     2.7352;
     2.6344;
     2.6094;
     2.3684;
     2.3222;
     2.2543;
     2.2099;
     2];
[ans, er, ifail] = d01ga(x, y)
ans =
   3.1414
er =
  -5.9352e-05
ifail =
```

[NP3663/21] d01ga.3 (last)