D01 – Quadrature d01fc

NAG Toolbox for MATLAB

1 Purpose

d01fc attempts to evaluate a multi-dimensional integral (up to 15 dimensions), with constant and finite limits, to a specified relative accuracy, using an adaptive subdivision strategy.

2 Syntax

```
[minpts, acc, finval, ifail] = d01fc(a, b, minpts, maxpts, functn, eps,
'ndim', ndim)
```

3 Description

d01fc returns an estimate of a multi-dimensional integral over a hyper-rectangle (i.e., with constant limits), and also an estimate of the relative error. You set the relative accuracy required, return values for the integrand via a function argument user-supplied real function **functn**, and also set the minimum and maximum acceptable number of calls to **functn** (in **minpts** and **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 co-ordinate axis are evaluated, and the subregion is marked for possible future subdivision in half along that co-ordinate 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 **minpts** calls to user-supplied real function **functn** 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 co-ordinate axis.

The function will fail if the requested relative error level has not been attained by the time **maxpts** calls to user-supplied real function **functn** have been made; or, if the amount **lenwrk** of working storage is insufficient. A formula for the recommended value of **lenwrk** is given in Section 5. If a smaller value is used, and is exhausted in the course of execution, the function switches to a less efficient mode of operation; only if this mode also breaks down is insufficient storage reported.

d01fc is based on the HALF (sub)program developed by van Dooren and De Ridder 1976. It uses a different basic rule, described in Genz and Malik 1980.

4 References

Genz A C and Malik A A 1980 An Adaptive Algorithm for Numerical Integration over an N-dimensional Rectangular Region *J. Comput. Appl. Math.* **6** 295–302

van Dooren P and De Ridder L 1976 An adaptive algorithm for numerical integration over an N-dimensional cube J. Comput. Appl. Math. 2 207–217

5 Parameters

5.1 Compulsory Input Parameters

1: **a(ndim) – double array**

The lower limits of integration, a_i , for i = 1, 2, ..., n.

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2: b(ndim) - double array

The upper limits of integration, b_i , for i = 1, 2, ..., n.

3: minpts - int32 scalar

Must be set to the minimum number of integrand evaluations to be allowed.

4: maxpts - int32 scalar

The maximum number of integrand evaluations to be allowed.

Constraints:

```
maxpts \ge minpts;
```

maxpts
$$\geq \alpha$$
, where $\alpha = 2^{\text{ndim}} + 2 \times \text{ndim}^2 + 2 \times \text{ndim} + 1$.

5: functn – string containing name of m-file

functn must return the value of the integrand f at a given point.

Its specification is:

```
[result] = functn(ndim, z)
```

Input Parameters

1: ndim – int32 scalar

n, the number of dimensions of the integral.

2: z(ndim) - double array

The co-ordinates of the point at which the integrand f must be evaluated.

Output Parameters

1: result – double scalar

The result of the function.

6: **eps – double scalar**

The relative error acceptable to you. When the solution is zero or very small relative accuracy may not be achievable but you may still set **eps** to a reasonable value and check for the error exit **ifail** = 2.

Constraint: eps > 0.0.

5.2 Optional Input Parameters

1: ndim – int32 scalar

Default: The dimension of the arrays \mathbf{a} , \mathbf{b} . (An error is raised if these dimensions are not equal.) n, the number of dimensions of the integral.

Constraint: $2 \le ndim \le 15$.

5.3 Input Parameters Omitted from the MATLAB Interface

lenwrk, wrkstr

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5.4 Output Parameters

1: minpts - int32 scalar

Contains the actual number of integrand evaluations used by d01fc.

2: acc – double scalar

The estimated relative error in finval.

3: finval – double scalar

The best estimate obtained for the integral.

4: ifail – int32 scalar

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

6 Error Indicators and Warnings

Note: d01fc may return useful information for one or more of the following detected errors or warnings.

ifail = 1

```
On entry, \mathbf{ndim} < 2, or \mathbf{ndim} > 15, or \mathbf{maxpts} is too small, or \mathbf{lenwrk} < 2 \times \mathbf{ndim} + 4, or \mathbf{eps} \le 0.0.
```

ifail = 2

maxpts was too small to obtain the required relative accuracy eps. On soft failure, finval and acc contain estimates of the integral and the relative error, but acc will be greater than eps.

ifail = 3

lenwrk was too small. On soft failure, finval and acc contain estimates of the integral and the relative error, but acc will be greater than eps.

7 Accuracy

A relative error estimate is output through the parameter acc.

8 Further Comments

Execution time will usually be dominated by the time taken to evaluate the user-supplied real function functn, and hence the maximum time that could be taken will be proportional to maxpts.

9 Example

```
d01fc_functn.m
function result = functn(ndim,z)
    result = 4.0*z(1)*z(3)*z(3)*exp(2.0*z(1)*z(3))/(1.0+z(2)+z(4))^2;

a = [0;
    0;
    0;
    0;
```

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```
0];
b = [1;
    1;
    1;
    1];
minpts = int32(0);
maxpts = int32(8000);
eps = 0.0001;
[minptsOut, acc, finval, ifail] = d01fc(a, b, minpts, maxpts,
'd01fc_functn', eps)

minptsOut =
    2223
acc =
    9.8932e-05
finval =
    0.5754
ifail =
    0
```

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