NAG Toolbox for MATLAB

d01pa

1 Purpose

d01pa returns a sequence of approximations to the integral of a function over a multi-dimensional simplex, together with an error estimate for the last approximation.

2 Syntax

```
[vert, minord, finvls, esterr, ifail] = d01pa(ndim, vert, functn,
minord, finvls, 'sdvert', sdvert, 'maxord', maxord)
```

3 Description

d01pa computes a sequence of approximations **finvls**(j), for $j = \mathbf{minord} + 1,\ \mathbf{minord} + 2, \ldots, \mathbf{maxord}$, to an integral

$$\int_S f(x_1, x_2, \ldots, x_n)\, dx_1 dx_2 \cdots dx_n$$

where S is an n-dimensional simplex defined in terms of its $n + 1$ vertices. **finvls**(j) is an approximation which will be exact (except for rounding errors) whenever the integrand is a polynomial of total degree $2j - 1$ or less.

The type of method used has been described in Grundmann and Moller 1978, and is implemented in an extrapolated form using the theory from de Doncker 1979.

4 References

de Doncker E 1979 New Euler–Maclaurin Expansions and their application to quadrature over the s-dimensional simplex *Math. Comput.* **33** 1003–1018

Grundmann A and Moller H M 1978 Invariant integration formulas for the n-simplex by combinatorial methods *SIAM J. Numer. Anal.* **15** 282–290

5 Parameters

5.1 Compulsory Input Parameters

1: **ndim – int32 scalar**

n, the number of dimensions of the integral.

Constraint: **ndim** ≥ 2.

2: **vert**(**ldvert,sdvert**) **– double array**

ldvert, the first dimension of the array, must be at least **ndim** $+ 1$.

vert(i,j) must be set to the jth component of the ith vertex for the simplex integration region, for $i = 1, 2, \ldots, n + 1$ and $j = 1, 2, \ldots, n$. If **minord** > 0, **vert** must be unchanged since the previous call of d01pa.

3: **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, x)
```

Input Parameters

1: **ndim – int32 scalar**

n, the number of dimensions of the integral.

2: **x(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.

4: **minord – int32 scalar**

Must specify the highest order of the approximations currently available in the array **finvls**. **minord** $= 0$ indicates an initial call; **minord** > 0 indicates that **finvls**(1), **finvls**(2), $\ldots$, **finvls**(**minord**) have already been computed in a previous call of d01pa.

Constraint: **minord** ≥ 0.

5: **finvls(maxord) – double array**

finvls(1), **finvls**(2), $\ldots$, **finvls**(**minord**) must contain approximations to the integral previously computed by d01pa.

5.2 Optional Input Parameters

1: **sdvert – int32 scalar**

Default: The second dimension of the array **vert**.

Constraint: **sdvert** $\geq 2 \times$ (**ndim** $+ 1$).

2: **maxord – int32 scalar**

Default: The dimension of the array **finvls**.

the highest order of approximation to the integral to be computed.

Constraint: **maxord** $>$ **minord**.

5.3 Input Parameters Omitted from the MATLAB Interface

ldvert

5.4 Output Parameters

1: **vert(ldvert,sdvert) – double array**

These values are unchanged. The rest of the array **vert** is used for workspace and contains information to be used if another call of d01pa is made with **minord** > 0. In particular **vert**$(n + 1, 2n + 2)$ contains the volume of the simplex.

2: **minord – int32 scalar**

minord $=$ **maxord**.

3: **finvls**(**maxord**) **– double array**

Contains these values unchanged, and the newly computed values **finvls**(**minord** + 1), **finvls**(**minord** + 2), . . . , **finvls**(**maxord**). **finvls**(j) is an approximation to the integral of polynomial degree $2j - 1$.

4: **esterr – double scalar**

An absolute error estimate for **finvls**(**maxord**).

5: **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

On entry, **ndim** < 2,
or **ldvert** < **ndim** + 1,
or **sdvert** < 2 × (**ndim** + 1),
or **minord** < 0,
or **maxord** ≤ **minord**.

ifail = 2

The volume of the simplex integration region (computed as a determinant by f03aa) is too large or too small to be representable in the machine.

7 Accuracy

An absolute error estimate is output through the parameter **esterr**.

8 Further Comments

The running time for d01pa will usually be dominated by the time used to evaluate the integrand user-supplied real function **functn**. The maximum time that could be used by d01pa will be approximately given by

$$T \times \frac{(\mathbf{maxord} + \mathbf{ndim})!}{(\mathbf{maxord} - 1)!(\mathbf{ndim} + 1)!}$$

where T is the time needed for one call of **functn**.

9 Example

d01pa_functn.m

```
function result = d01pa_functn(ndim, x)
  result = exp(x(1)+x(2)+x(3))*cos(x(1)+x(2)+x(3));
```

```
ndim = int32(3);
vertex = [0, 0, 0, 0, 0, 0, 0, 0;
     1, 0, 0, 0, 0, 0, 0, 0;
     0, 1, 0, 0, 0, 0, 0, 0;
     0, 0, 1, 0, 0, 0, 0, 0];
minord = int32(0);
```

```
finvls = [0];
[vertexOut, minordOut, finvlsOut, esterr, ifail] = ...
    d01pa(ndim, vertex, 'd01pa_functn', minord, finvls)
```

```
vertexOut =
  Columns 1 through 7
         0         0         0         0         0   -0.5000         0
    1.0000         0         0    0.5000         0   -0.5000         0
         0    1.0000         0         0    0.5000   -0.5000         0
         0         0    1.0000         0         0         0    3.0000
  Column 8
    0.2500
    0.2500
    0.2500
    1.0000
minordOut =
           1
finvlsOut =
    0.2582
esterr =
    0.2582
ifail =
           0
```