

# NAG Library Routine Document

## D01FBF

**Note:** before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details.

### 1 Purpose

D01FBF computes an estimate of a multidimensional integral (from 1 to 20 dimensions), given the analytic form of the integrand and suitable Gaussian weights and abscissae.

### 2 Specification

FUNCTION D01FBF (NDIM, NPTVEC, LWA, WEIGHT, ABCSIS, FUN, IFAIL)

REAL (KIND=nag\_wp) D01FBF

INTEGER NDIM, NPTVEC(NDIM), LWA, IFAIL

REAL (KIND=nag\_wp) WEIGHT(LWA), ABCSIS(LWA), FUN

EXTERNAL FUN

### 3 Description

D01FBF approximates a multidimensional integral by evaluating the summation

$$\sum_{i_1=1}^{l_1} w_{1,i_1} \sum_{i_2=1}^{l_2} w_{2,i_2} \cdots \sum_{i_n=1}^{l_n} w_{n,i_n} f(x_{1,i_1}, x_{2,i_2}, \dots, x_{n,i_n})$$

given the weights  $w_{j,i_j}$  and abscissae  $x_{j,i_j}$  for a multidimensional product integration rule (see Davis and Rabinowitz (1975)). The number of dimensions may be anything from 1 to 20.

The weights and abscissae for each dimension must have been placed in successive segments of the arrays WEIGHT and ABCSIS; for example, by calling D01BCF or D01TBF once for each dimension using a quadrature formula and number of abscissae appropriate to the range of each  $x_j$  and to the functional dependence of  $f$  on  $x_j$ .

If normal weights are used, the summation will approximate the integral

$$\int w_1(x_1) \int w_2(x_2) \cdots \int w_n(x_n) f(x_1, x_2, \dots, x_n) dx_n \cdots dx_2 dx_1$$

where  $w_j(x)$  is the weight function associated with the quadrature formula chosen for the  $j$ th dimension; while if adjusted weights are used, the summation will approximate the integral

$$\int \int \cdots \int f(x_1, x_2, \dots, x_n) dx_n \cdots dx_2 dx_1.$$

You must supply a subroutine to evaluate

$$f(x_1, x_2, \dots, x_n)$$

at any values of  $x_1, x_2, \dots, x_n$  within the range of integration.

### 4 References

Davis P J and Rabinowitz P (1975) *Methods of Numerical Integration* Academic Press

## 5 Parameters

- 1: NDIM – INTEGER *Input*  
*On entry:*  $n$ , the number of dimensions of the integral.  
*Constraint:*  $1 \leq \text{NDIM} \leq 20$ .
- 2: NPTVEC(NDIM) – INTEGER array *Input*  
*On entry:* NPTVEC( $j$ ) must specify the number of points in the  $j$ th dimension of the summation, for  $j = 1, 2, \dots, n$ .
- 3: LWA – INTEGER *Input*  
*On entry:* the dimension of the arrays WEIGHT and ABSCIS as declared in the (sub)program from which D01FBB is called.  
*Constraint:*  $\text{LWA} \geq \text{NPTVEC}(1) + \text{NPTVEC}(2) + \dots + \text{NPTVEC}(\text{NDIM})$ .
- 4: WEIGHT(LWA) – REAL (KIND=nag\_wp) array *Input*  
*On entry:* must contain in succession the weights for the various dimensions, i.e., WEIGHT( $k$ ) contains the  $i$ th weight for the  $j$ th dimension, with
- $$k = \text{NPTVEC}(1) + \text{NPTVEC}(2) + \dots + \text{NPTVEC}(j - 1) + i.$$
- 5: ABSCIS(LWA) – REAL (KIND=nag\_wp) array *Input*  
*On entry:* must contain in succession the abscissae for the various dimensions, i.e., ABSCIS( $k$ ) contains the  $i$ th abscissa for the  $j$ th dimension, with
- $$k = \text{NPTVEC}(1) + \text{NPTVEC}(2) + \dots + \text{NPTVEC}(j - 1) + i.$$
- 6: FUN – REAL (KIND=nag\_wp) FUNCTION, supplied by the user. *External Procedure*  
 FUN must return the value of the integrand  $f$  at a specified point.

The specification of FUN is:

```
FUNCTION FUN (NDIM, X)
  REAL (KIND=nag_wp) FUN
  INTEGER          NDIM
  REAL (KIND=nag_wp) X(NDIM)
```

- 1: NDIM – INTEGER *Input*  
*On entry:*  $n$ , the number of dimensions of the integral.
- 2: X(NDIM) – REAL (KIND=nag\_wp) array *Input*  
*On entry:* the coordinates of the point at which the integrand  $f$  must be evaluated.

FUN must either be a module subprogram USED by, or declared as EXTERNAL in, the (sub)program from which D01FBB is called. Parameters denoted as *Input* must **not** be changed by this procedure.

- 7: IFAIL – INTEGER *Input/Output*  
*On entry:* IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this parameter, the

recommended value is 0. **When the value  $-1$  or  $1$  is used it is essential to test the value of IFAIL on exit.**

*On exit:* IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

## 6 Error Indicators and Warnings

If on entry IFAIL = 0 or  $-1$ , explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL = 1

On entry, NDIM < 1,  
or NDIM > 20,  
or LWA < NPTVEC(1) + NPTVEC(2) +  $\dots$  + NPTVEC(NDIM).

## 7 Accuracy

The accuracy of the computed multidimensional sum depends on the weights and the integrand values at the abscissae. If these numbers vary significantly in size and sign then considerable accuracy could be lost. If these numbers are all positive, then little accuracy will be lost in computing the sum.

## 8 Further Comments

The total time taken by D01FBF will be proportional to

$$T \times \text{NPTVEC}(1) \times \text{NPTVEC}(2) \times \dots \times \text{NPTVEC}(\text{NDIM}),$$

where  $T$  is the time taken for one evaluation of FUN.

## 9 Example

This example evaluates the integral

$$\int_1^2 \int_0^\infty \int_{-\infty}^\infty \int_1^\infty \frac{(x_1 x_2 x_3)^6}{(x_4 + 2)^8} e^{-2x_2} e^{-0.5x_3^2} dx_4 dx_3 dx_2 dx_1$$

using adjusted weights. The quadrature formulae chosen are:

$x_1$ : Gauss–Legendre,  $a = 1.0$ ,  $b = 2.0$ ,

$x_2$ : Gauss–Laguerre,  $a = 0.0$ ,  $b = 2.0$ ,

$x_3$ : Gauss–Hermite,  $a = 0.0$ ,  $b = 0.5$ ,

$x_4$ : rational Gauss,  $a = 1.0$ ,  $b = 2.0$ .

Four points are sufficient in each dimension, as this integral is in fact a product of four one-dimensional integrals, for each of which the chosen four-point formula is exact.

### 9.1 Program Text

```
! D01FBF Example Program Text
! Mark 24 Release. NAG Copyright 2012.

Module d01fbfe_mod

! D01FBF Example Program Module:
! Parameters and User-defined Routines

! .. Use Statements ..
Use nag_library, Only: nag_wp
```

```

! .. Implicit None Statement ..
Implicit None
! .. Parameters ..
Integer, Parameter :: ndim = 4, nout = 6
Contains
Function fun(ndim,x)

! .. Function Return Value ..
Real (Kind=nag_wp) :: fun
! .. Scalar Arguments ..
Integer, Intent (In) :: ndim
! .. Array Arguments ..
Real (Kind=nag_wp), Intent (In) :: x(ndim)
! .. Intrinsic Procedures ..
Intrinsic :: exp
! .. Executable Statements ..
fun = (x(1)*x(2)*x(3))**6/(x(4)+2.0E0_nag_wp)**8* &
exp(-2.0E0_nag_wp*x(2)-0.5E0_nag_wp*x(3)*x(3))

Return

End Function fun
End Module d01fbfe_mod
Program d01fbfe

! D01FBF Example Main Program

! .. Use Statements ..
Use nag_library, Only: d01baw, d01bax, d01bay, d01baz, d01bbf, d01fbf, &
nag_wp
Use d01fbfe_mod, Only: fun, ndim, nout
! .. Implicit None Statement ..
Implicit None
! .. Local Scalars ..
Real (Kind=nag_wp) :: a, ans, b
Integer :: i, ifail, itype, j, lwa
! .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: abscis(:), weight(:)
Integer :: nptvec(ndim)
! .. Intrinsic Procedures ..
Intrinsic :: sum
! .. Executable Statements ..
Write (nout,*) 'D01FBF Example Program Results'

nptvec(1:ndim) = (/4,4,4,4/)
lwa = sum(nptvec(1:ndim))
Allocate (abscis(lwa),weight(lwa))

itype = 1
j = 1

Do i = 1, 4

    ifail = 0
    Select Case (i)
    Case (1)
        a = 1.0E0_nag_wp
        b = 2.0E0_nag_wp
        Call d01bbf(d01baz,a,b,itype,nptvec(i),weight(j),abscis(j),ifail)
    Case (2)
        a = 0.0E0_nag_wp
        b = 2.0E0_nag_wp
        Call d01bbf(d01bax,a,b,itype,nptvec(i),weight(j),abscis(j),ifail)
    Case (3)
        a = 0.0E0_nag_wp
        b = 0.5E0_nag_wp
        Call d01bbf(d01baw,a,b,itype,nptvec(i),weight(j),abscis(j),ifail)
    Case (4)
        a = 1.0E0_nag_wp
        b = 2.0E0_nag_wp
        Call d01bbf(d01bay,a,b,itype,nptvec(i),weight(j),abscis(j),ifail)
    
```

```
      End Select
      j = j + nptvec(i)
    End Do

    ifail = 0
    ans = d01fbf(ndim,nptvec,lwa,weight,abscis,fun,ifail)

    Write (nout,*)
    Write (nout,99999) 'Answer = ', ans

99999 Format (1X,A,F10.5)
End Program d01fbfe
```

## 9.2 Program Data

None.

## 9.3 Program Results

D01FBF Example Program Results

Answer = 0.25065

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