

# NAG Library Routine Document

## D01GYF

**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

D01GYF calculates the optimal coefficients for use by D01GCF and D01GDF, for prime numbers of points.

### 2 Specification

```
SUBROUTINE D01GYF (NDIM, NPTS, VK, IFAIL)
  INTEGER          NDIM, NPTS, IFAIL
  REAL (KIND=nag_wp) VK(NDIM)
```

### 3 Description

The Korobov (1963) procedure for calculating the optimal coefficients  $a_1, a_2, \dots, a_n$  for  $p$ -point integration over the  $n$ -cube  $[0, 1]^n$  imposes the constraint that

$$a_1 = 1 \quad \text{and} \quad a_i = a^{i-1} \pmod{p}, \quad i = 1, 2, \dots, n \quad (1)$$

where  $p$  is a prime number and  $a$  is an adjustable argument. This argument is computed to minimize the error in the integral

$$3^n \int_0^1 dx_1 \cdots \int_0^1 dx_n \prod_{i=1}^n (1 - 2x_i)^2, \quad (2)$$

when computed using the number theoretic rule, and the resulting coefficients can be shown to fit the Korobov definition of optimality.

The computation for large values of  $p$  is extremely time consuming (the number of elementary operations varying as  $p^2$ ) and there is a practical upper limit to the number of points that can be used. Routine D01GZF is computationally more economical in this respect but the associated error is likely to be larger.

### 4 References

Korobov N M (1963) *Number Theoretic Methods in Approximate Analysis* Fizmatgiz, Moscow

### 5 Arguments

- |    |  |               |
|----|--|---------------|
| 1: | NDIM – INTEGER   | <i>Input</i>  |
|    | <i>On entry:</i> $n$ , the number of dimensions of the integral. |               |
|    | <i>Constraint:</i> $\text{NDIM} \geq 1$ .                        |               |
| 2: | NPTS – INTEGER   | <i>Input</i>  |
|    | <i>On entry:</i> $p$ , the number of points to be used.          |               |
|    | <i>Constraint:</i> NPTS must be a prime number $\geq 5$ .        |               |
| 3: | VK(NDIM) – REAL (KIND=nag_wp) array                              | <i>Output</i> |
|    | <i>On exit:</i> the $n$ optimal coefficients.                    |               |

## 4: IFAIL – INTEGER

*Input/Output*

*On entry:* IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation 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 argument, 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.

IFAIL = 2

On entry, NPTS < 5.

IFAIL = 3

On entry, NPTS is not a prime number.

IFAIL = 4

The precision of the machine is insufficient to perform the computation exactly. Try a smaller value of NPTS, or use an implementation of higher precision.

IFAIL = -99

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

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -399

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

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

## 7 Accuracy

The optimal coefficients are returned as exact integers (though stored in a real array).

## 8 Parallelism and Performance

D01GYF is not threaded in any implementation.

## 9 Further Comments

The time taken is approximately proportional to  $p^2$  (see Section 3).

## 10 Example

This example calculates the Korobov optimal coefficients where the number of dimensions is 4 and the number of points is 631.

### 10.1 Program Text

```

Program d01gyfe

!      D01GYF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
      Use nag_library, Only: d01gyf, nag_wp
!      .. Implicit None Statement ..
      Implicit None
!      .. Parameters ..
      Integer, Parameter          :: ndim = 4, nout = 6
!      .. Local Scalars ..
      Integer                     :: ifail, npts
!      .. Local Arrays ..
      Real (Kind=nag_wp)         :: vk(20)
!      .. Executable Statements ..
      Write (nout,*) 'D01GYF Example Program Results'

      npts = 631

      ifail = 0
      Call d01gyf(ndim,npts,vk,ifail)

      Write (nout,*)
      Write (nout,99999) 'NDIM =', ndim, ' NPTS =', npts
      Write (nout,*)
      Write (nout,99998) 'Coefficients =', vk(1:ndim)

99999 Format (1X,A,I3,A,I6)
99998 Format (1X,A,4F6.0)
End Program d01gyfe

```

### 10.2 Program Data

None.

### 10.3 Program Results

```

D01GYF Example Program Results

NDIM =   4 NPTS =   631

Coefficients =    1.  198.   82.  461.

```

---