

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
double precision VK(NDIM)
```

3 Description

The Korobov procedure Korobov (1963) 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 parameter. This parameter 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 Parameters

- | | | |
|----|--|---------------|
| 1: | NDIM – INTEGER | <i>Input</i> |
| | <i>On entry:</i> n , the number of dimensions of the integral. | |
| | <i>Constraint:</i> 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) – <i>double precision</i> 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 parameter you should refer to Section 3.3 in the Essential Introduction for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

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.**

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.

7 Accuracy

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

8 Further Comments

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

9 Example

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

9.1 Program Text

```
*      D01GYF Example Program Text
*      Mark 14 Revised. NAG Copyright 1989.
*      .. Parameters ..
      INTEGER          NDIM
      PARAMETER        (NDIM=4)
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*      .. Local Scalars ..
      INTEGER          I, IFAIL, NPTS
*      .. Local Arrays ..
      DOUBLE PRECISION VK(20)
*      .. External Subroutines ..
```

```
EXTERNAL          D01GYF
* .. Executable Statements ..
WRITE (NOUT,*) 'D01GYF Example Program Results'
NPTS = 631
WRITE (NOUT,*)
IFAIL = 1
*
CALL D01GYF(NDIM,NPTS,VK,IFAIL)
*
IF (IFAIL.EQ.0) THEN
  WRITE (NOUT,99999) 'NDIM =', NDIM, ' NPTS =', NPTS
  WRITE (NOUT,*)
  WRITE (NOUT,99998) 'Coefficients =', (VK(I),I=1,NDIM)
ELSE
  WRITE (NOUT,99997) ' ** D01GYF returned with IFAIL = ', IFAIL
END IF
*
99999 FORMAT (1X,A,I3,A,I6)
99998 FORMAT (1X,A,4F6.0)
99997 FORMAT (1X,A,I5)
END
```

9.2 Program Data

None.

9.3 Program Results

```
D01GYF Example Program Results
NDIM = 4 NPTS = 631
Coefficients = 1. 198. 82. 461.
```
