D01GYF – NAG Fortran Library Routine Document

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              VK(NDIM)
```

3 Description

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

$$\begin{aligned} a_1 &= 1 \\ a_i &= a^{i-1} \pmod{p}, \qquad i = 1, 2, \ldots, n \end{aligned} \tag{1}$$

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

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

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

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

5 Parameters

1: NDIM — INTEGER *Input*

On entry: the number of dimensions of the integral, n.

Constraint: NDIM ≥ 1.

2: NPTS — INTEGER *Input*

On entry: the number of points to be used, p.

Constraint: NPTS must be a prime number ≥ 5.

3: VK(NDIM) — ***real*** array *Output*

On exit: the n optimal coefficients.

4: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, −1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

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

6 Error Indicators and Warnings

Errors 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 program calculates the Korobov optimal coefficients where the number of dimensions is 4 and the number of points is 631.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     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 ..
      real             VK(20)
*     .. External Subroutines ..
      EXTERNAL         D01GYF
```

```
*     .. Executable Statements ..
      WRITE (NOUT,*) 'D01GYF Example Program Results'
      NPTS = 631
      WRITE (NOUT,*)
      WRITE (NOUT,99999) 'NDIM =', NDIM, ' NPTS =', NPTS
      IFAIL = 0
*
      CALL D01GYF(NDIM,NPTS,VK,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,99998) 'Coefficients =', (VK(I),I=1,NDIM)
      STOP
*
99999 FORMAT (1X,A,I3,A,I6)
99998 FORMAT (1X,A,4F6.0)
      END
```

9.2 Program Data

None.

9.3 Program Results

```
 D01GYF Example Program Results

 NDIM =  4 NPTS =   631

 Coefficients =    1.  198.   82.  461.
```