

# NAG Library Routine Document

## G01LBF

**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

G01LBF returns a number of values of the probability density function (PDF), or its logarithm, for the multivariate Normal (Gaussian) distribution.

### 2 Specification

SUBROUTINE G01LBF (ILOG, K, N, X, LDX, XMU, IULD, SIG, LDSIG, PDF, RANK, &  
IFAIL)

INTEGER ILOG, K, N, LDX, IULD, LDSIG, RANK, IFAIL  
REAL (KIND=nag\_wp) X(LDX,\*), XMU(N), SIG(LDSIG,\*), PDF(K)

### 3 Description

The probability density function,  $f(X : \mu, \Sigma)$  of an  $n$ -dimensional multivariate Normal distribution with mean vector  $\mu$  and  $n$  by  $n$  variance-covariance matrix  $\Sigma$ , is given by

$$f(X : \mu, \Sigma) = ((2\pi)^n |\Sigma|)^{-1/2} \exp\left(-\frac{1}{2}(X - \mu)^T \Sigma^{-1}(X - \mu)\right).$$

If the variance-covariance matrix,  $\Sigma$ , is not of full rank then the probability density function, is calculated as

$$f(X : \mu, \Sigma) = ((2\pi)^r \text{pdet}(\Sigma))^{-1/2} \exp\left(-\frac{1}{2}(X - \mu)^T \Sigma^-(X - \mu)\right)$$

where  $\text{pdet}(\Sigma)$  is the pseudo-determinant,  $\Sigma^-$  a generalized inverse of  $\Sigma$  and  $r$  its rank.

G01LBF evaluates the PDF at  $k$  points with a single call.

### 4 References

None.

### 5 Arguments

1: ILOG – INTEGER *Input*

*On entry:* the value of ILOG determines whether the logarithmic value is returned in PDF.

ILOG = 0

$f(X : \mu, \Sigma)$ , the probability density function is returned.

ILOG = 1

$\log(f(X : \mu, \Sigma))$ , the logarithm of the probability density function is returned.

*Constraint:* ILOG = 0 or 1.

2: K – INTEGER *Input*

*On entry:*  $k$ , the number of points the PDF is to be evaluated at.

*Constraint:*  $K \geq 0$ .

- 3: N – INTEGER *Input*  
*On entry:*  $n$ , the number of dimensions.  
*Constraint:*  $N \geq 2$ .
- 4: X(LDX,\*) – REAL (KIND=nag\_wp) array *Input*  
**Note:** the second dimension of the array X must be at least K.  
*On entry:* X, the matrix of  $k$  points at which to evaluate the probability density function, with the  $i$ th dimension for the  $j$ th point held in  $X(i, j)$ .
- 5: LDX – INTEGER *Input*  
*On entry:* the first dimension of the array X as declared in the (sub)program from which G01LBF is called.  
*Constraint:*  $LDX \geq N$ .
- 6: XMU(N) – REAL (KIND=nag\_wp) array *Input*  
*On entry:*  $\mu$ , the mean vector of the multivariate Normal distribution.
- 7: IULD – INTEGER *Input*  
*On entry:* indicates the form of  $\Sigma$  and how it is stored in SIG.  
 IULD = 1  
     SIG holds the lower triangular portion of  $\Sigma$ .  
 IULD = 2  
     SIG holds the upper triangular portion of  $\Sigma$ .  
 IULD = 3  
      $\Sigma$  is a diagonal matrix and SIG only holds the diagonal elements.  
 IULD = 4  
     SIG holds the lower Cholesky decomposition,  $L$  such that  $LL^T = \Sigma$ .  
 IULD = 5  
     SIG holds the upper Cholesky decomposition,  $U$  such that  $U^TU = \Sigma$ .  
*Constraint:* IULD = 1, 2, 3, 4 or 5.
- 8: SIG(LDSIG,\*) – REAL (KIND=nag\_wp) array *Input*  
**Note:** the second dimension of the array SIG must be at least N.  
*On entry:* information defining the variance-covariance matrix,  $\Sigma$ .  
 IULD = 1 or 2  
     SIG must hold the lower or upper portion of  $\Sigma$ , with  $\Sigma_{ij}$  held in  $SIG(i, j)$ . The supplied variance-covariance matrix must be positive semidefinite.  
 IULD = 3  
      $\Sigma$  is a diagonal matrix and the  $i$ th diagonal element,  $\Sigma_{ii}$ , must be held in  $SIG(1, i)$   
 IULD = 4 or 5  
     SIG must hold  $L$  or  $U$ , the lower or upper Cholesky decomposition of  $\Sigma$ , with  $L_{ij}$  or  $U_{ij}$  held in  $SIG(i, j)$ , depending on the value of IULD. No check is made that  $LL^T$  or  $U^TU$  is a valid variance-covariance matrix. The diagonal elements of the supplied  $L$  or  $U$  must be greater than zero
- 9: LDSIG – INTEGER *Input*  
*On entry:* the first dimension of the array SIG as declared in the (sub)program from which G01LBF is called.

*Constraints:*

if IULD = 3, LDSIG  $\geq$  1;  
otherwise LDSIG  $\geq$  N.

10: PDF(K) – REAL (KIND=nag\_wp) array *Output*

*On exit:*  $f(X : \mu, \Sigma)$  or  $\log(f(X : \mu, \Sigma))$  depending on the value of ILOG.

11: RANK – INTEGER *Output*

*On exit:*  $r$ , rank of  $\Sigma$ .

12: 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 = 11

On entry, ILOG =  $\langle value \rangle$ .  
Constraint: ILOG = 0 or 1.

IFAIL = 21

On entry, K =  $\langle value \rangle$ .  
Constraint:  $K \geq 0$ .

IFAIL = 31

On entry, N =  $\langle value \rangle$ .  
Constraint:  $N \geq 2$ .

IFAIL = 51

On entry, LDX =  $\langle value \rangle$  and N =  $\langle value \rangle$ .  
Constraint:  $LDX \geq N$ .

IFAIL = 71

On entry, IULD =  $\langle value \rangle$ .  
Constraint: IULD = 1, 2, 3, 4 or 5.

IFAIL = 81

On entry,  $\Sigma$  is not positive semidefinite.

IFAIL = 82

On entry, at least one diagonal element of  $\Sigma$  is less than or equal to 0.

IFAIL = 83

On entry,  $\Sigma$  is not positive definite and eigenvalue decomposition failed.

IFAIL = 91

On entry, LDSIG = *value*.

Constraint: if IULD = 3, LDSIG  $\geq$  1.

IFAIL = 92

On entry, LDSIG = *value*.

Constraint: if IULD  $\neq$  3, LDSIG  $\geq$  N.

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

Not applicable.

## 8 Parallelism and Performance

G01LBF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

G01LBF makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

## 9 Further Comments

None.

## 10 Example

This example prints the value of the multivariate Normal PDF at a number of different points.

**10.1 Program Text**

```

Program g01lbfe

!      G01LBF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
Use nag_library, Only: g01lbfe, nag_wp, x04caf
!      .. Implicit None Statement ..
Implicit None
!      .. Parameters ..
Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
Integer                     :: i, ifail, ilog, iuld, k, ldsig, ldx, &
                             n, rank
!      .. Local Arrays ..
Real (Kind=nag_wp), Allocatable :: pdf(:), sig(:,,:), x(:,,:), xmu(:)
!      .. Intrinsic Procedures ..
Intrinsic                   :: repeat
!      .. Executable Statements ..
Write (nout,*) 'G01LBF Example Program Results'
Write (nout,*)
Flush (nout)

!      Skip heading in data file
Read (nin,*)

!      Read in the problem size and how the covariance matrix is stored
!      and whether the log PDF is required
Read (nin,*) k, n, iuld, ilog

!      Allocate arrays
ldx = n
Allocate (x(ldx,k),xmu(n),pdf(k))

!      Read in and echo the vector of means
Read (nin,*) xmu(1:n)
Write (nout,*) 'Vector of Means: '
Write (nout,99999) xmu(1:n)
Write (nout,*)

!      Read in and echo the covariance matrix
If (iuld==3) Then
!      Covariance matrix is diagonal
ldsig = 1
Allocate (sig(ldsig,n))
Read (nin,*) sig(1,1:n)

Write (nout,*) 'Diagonal Elements of Covariance Matrix: '
Write (nout,99999) sig(1,1:n)

Else
!      Read in an upper or lower triangular matrix
ldsig = n
Allocate (sig(ldsig,n))
If (iuld==1 .Or. iuld==4) Then
!      Lower triangular matrix
Read (nin,*)(sig(i,1:i),i=1,n)

If (iuld==1) Then
Call x04caf('Lower','Nonunit',n,n,sig,ldsig,'Covariance Matrix:', &
ifail)
Else
Call x04caf('Lower','Nonunit',n,n,sig,ldsig, &
'Lower Triangular Cholesky Factor of Covariance Matrix:',ifail)
End If
Else
!      Upper triangular matrix
Read (nin,*)(sig(i,i:n),i=1,n)

```

```

      If (iuld==2) Then
        Call x04caf('Upper','Nonunit',n,n,sig,ldsig,'Covariance Matrix:', &
          ifail)
      Else
        Call x04caf('Upper','Nonunit',n,n,sig,ldsig,
          'Upper Triangular Cholesky Factor of Covariance Matrix:',ifail) &
      End If
    End If
  End If
End If

!   Read in the points at which to evaluate the PDF
Read (nin,*)(x(1:n,i),i=1,k)

!   Evaluate the PDF
ifail = 0
Call g01lbf(iolog,k,n,x,ldx,xmu,iuld,sig,ldsig,pdf,rank,ifail)

!   Display results
Write (nout,*)
Write (nout,*) 'Rank of the covariance matrix: ', rank
Write (nout,*)
If (iolog==1) Then
  Write (nout,*) '      log(PDF)                X'
Else
  Write (nout,*) '      PDF                    X'
End If
Write (nout,*) ' ', repeat('-',48)
Do i = 1, k
  Write (nout,99998) pdf(i), x(1:n,i)
End Do

99999 Format (1X,100(F8.4,1X))
99998 Format (1X,1P,E13.4,0P,10(1X,F8.4))
End Program g01lbfe

```

## 10.2 Program Data

```

G01LBF Example Program Data
  2  4  1  0      : K,N,IULD,ILOG
  0.10  0.20  0.30  0.40 : End XMU
  4.16
 -3.12  5.03
  0.56 -0.83  0.76
 -0.10  1.18  0.34  1.18 : End SIG
  1.00  1.00  1.00  1.00
  1.00  2.00  3.00  4.00 : End of X

```

## 10.3 Program Results

G01LBF Example Program Results

Vector of Means:  
 0.1000 0.2000 0.3000 0.4000

Covariance Matrix:

	1	2	3	4
1	4.1600			
2	-3.1200	5.0300		
3	0.5600	-0.8300	0.7600	
4	-0.1000	1.1800	0.3400	1.1800

Rank of the covariance matrix: 4

	PDF	X			
	3.0307E-03	1.0000	1.0000	1.0000	1.0000
	4.5232E-06	1.0000	2.0000	3.0000	4.0000

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