# NAG Library Routine Document <br> G03BDF 

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

G03BDF calculates a ProMax rotation, given information following an orthogonal rotation.

## 2 Specification

```
SUBROUTINE GO3BDF (STAND, N, M, X, LDX, RO, LDRO, POWER, FP, LDFP, R,
    LDR, PHI, LDPHI, FS, LDFS, IFAIL)
INTEGER N, M, LDX, LDRO, LDFP, LDR, LDPHI, LDFS, IFAIL
REAL (KIND=nag_wp) X (LDX,M), RO(LDRO,M), POWER, FP(LDFP,M), R(LDR,M), &
    PHI(LDPHI,M), FS(LDFS,M)
CHARACTER(1) STAND
```


## 3 Description

Let $X$ and $Y$ denote $n$ by $m$ matrices each representing a set of $n$ points in an $m$-dimensional space. The $X$ matrix is a matrix of loadings as returned by G03BAF, that is following an orthogonal rotation of a loadings matrix $Z$. The target matrix $Y$ is calculated as a power transformation of $X$ that preserves the sign of the loadings. Let $X_{i j}$ and $Y_{i j}$ denote the $(i, j)$ th element of matrices $X$ and $Y$. Given a value greater than one for the exponent $p$ :

$$
Y_{i j}=\delta_{i j}\left\|X_{i j}\right\|^{p}
$$

for

$$
\begin{aligned}
& i=1,2, \ldots, n \\
& j=1,2, \ldots, m \\
& \delta_{i j}=\left\{\begin{array}{r}
-1, \\
1, \\
1, \text { if } X_{i j}<0
\end{array}\right. \\
& \text { otherwise } .
\end{aligned}
$$

The above power transformation tends to increase the difference between high and low values of loadings and is intended to increase the interpretability of a solution.

In the second step a solution of:

$$
X W=Y, \quad X, Y \in \mathbb{R}^{n \times m}, W \in \mathbb{R}^{m \times m}
$$

is found for $W$ in the least squares sense by use of singular value decomposition of the orthogonal loadings $X$. The ProMax rotation matrix $R$ is then given by

$$
R=O W \tilde{W}, \quad O, \tilde{W} \in \mathbb{R}^{m \times m}
$$

where $O$ is the rotation matrix from an orthogonal transformation, and $\tilde{W}$ is a matrix with the square root of diagonal elements of $\left(W^{\mathrm{T}} W\right)^{-1}$ on its diagonal and zeros elsewhere.

The ProMax factor pattern matrix $P$ is given by

$$
P=X W \tilde{W}, \quad P \in \mathbb{R}^{n \times m}
$$

the inter-factor correlations $\Phi$ are given by

$$
\Phi=\left(Q^{\mathrm{T}} Q\right)^{-1}, \quad \Phi \in \mathbb{R}^{m \times m}
$$

where $Q=W \tilde{W}$; and the factor structure $S$ is given by

$$
S=P \Phi, \quad S \in \mathbb{R}^{n \times m}
$$

Optionally, the rows of target matrix $Y$ can be scaled by the communalities of loadings.

## 4 References

None.

## 5 Parameters

1: STAND - CHARACTER(1)
Input
On entry: indicates how loadings are normalized.
STAND = 'S'
Rows of $Y$ are (Kaiser) normalized by the communalities of the loadings.
STAND = 'U'
Rows are not normalized.
Constraint: STAND = 'U' or 'S'.
2: N - INTEGER Input
On entry: $n$, the number of points.
Constraint: $\mathrm{N} \geq \mathrm{M}$.
3: M - INTEGER
Input
On entry: $m$, the number of dimensions.
Constraint: $\mathrm{M} \geq 1$.

4: $\quad \mathrm{X}(\mathrm{LDX}, \mathrm{M})-\mathrm{REAL}(\mathrm{KIND}=$ nag_wp $)$ array
On entry: the loadings matrix following an orthogonal rotation, $X$.
5: LDX - INTEGER Input

On entry: the first dimension of the array X as declared in the (sub)program from which G03BDF is called.

Constraint: LDX $\geq \mathrm{N}$.
6: $\quad \mathrm{RO}(\mathrm{LDRO}, \mathrm{M})-\mathrm{REAL}(\mathrm{KIND}=$ nag_wp $)$ array
Input
On entry: the orthogonal rotation matrix, $O$.

7: LDRO - INTEGER
On entry: the first dimension of the array RO as declared in the (sub)program from which G 03 BDF is called.

Constraint: $\mathrm{LDRO} \geq \mathrm{M}$.

8: POWER - REAL (KIND=nag_wp) Input
On entry: $p$, the value of exponent.
Constraint: POWER > 1.0.

9: $\quad \mathrm{FP}(\mathrm{LDFP}, \mathrm{M})-$ REAL (KIND=$=$ nag_wp $)$ array
Output
On exit: the factor pattern matrix, $P$.

10: LDFP - INTEGER Input
On entry: the first dimension of the array FP as declared in the (sub)program from which G03BDF is called.

Constraint: $\mathrm{LDFP} \geq \mathrm{N}$.
11: $\quad \mathrm{R}(\mathrm{LDR}, \mathrm{M})-\mathrm{REAL}(\mathrm{KIND}=$ nag_wp) array
Output
On exit: the ProMax rotation matrix, $R$.

12: LDR - INTEGER
Input
On entry: the first dimension of the array R as declared in the (sub)program from which G03BDF is called.

Constraint: LDR $\geq \mathrm{M}$.
13: $\quad \operatorname{PHI}(\mathrm{LDPHI}, \mathrm{M})-\mathrm{REAL}(\mathrm{KIND}=$ nag_wp $)$ array
Output
On exit: the matrix of inter-factor correlations, $\Phi$.
14: LDPHI - INTEGER
Input
On entry: the first dimension of the array PHI as declared in the (sub)program from which G 03 BDF is called.

Constraint: $\mathrm{LDPHI} \geq \mathrm{M}$.
15: $\quad$ FS(LDFS, M) - REAL (KIND=nag_wp) array
Output
On exit: the factor structure matrix, $S$.

16: LDFS - INTEGER
Input
On entry: the first dimension of the array FS as declared in the (sub)program from which G03BDF is called.

Constraint: LDFS $\geq \mathrm{N}$.
17: 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, $\mathrm{M}=\langle$ value $\rangle$.
Constraint: $\mathrm{M} \geq 1$.

On entry, POWER $=\langle$ value $\rangle$.
Constraint: POWER > 1.0 .
On entry, STAND $=\langle$ value $\rangle$.
Constraint: STAND = 'U' or 'S'.
IFAIL $=2$
On entry, LDFP $=\langle$ value $\rangle$ and $\mathrm{N}=\langle$ value $\rangle$.
Constraint: LDFP $\geq \mathrm{N}$.
On entry, LDFS $=\langle$ value $\rangle$ and $\mathrm{N}=\langle$ value $\rangle$.
Constraint: LDFS $\geq \mathrm{N}$.
On entry, LDPHI $=\langle$ value $\rangle$ and $\mathrm{M}=\langle$ value $\rangle$.
Constraint: $\mathrm{LDPHI} \geq \mathrm{M}$.
On entry, $\mathrm{LDR}=\langle$ value $\rangle$ and $\mathrm{M}=\langle$ value $\rangle$.
Constraint: $\mathrm{LDR} \geq \mathrm{M}$.
On entry, $\mathrm{LDRO}=\langle$ value $\rangle$ and $\mathrm{M}=\langle$ value $\rangle$.
Constraint: $\mathrm{LDRO} \geq \mathrm{M}$.
On entry, $\mathrm{LDX}=\langle$ value $\rangle$ and $\mathrm{N}=\langle$ value $\rangle$.
Constraint: LDX $\geq \mathrm{N}$.
On entry, $\mathrm{N}=\langle$ value $\rangle$ and $\mathrm{M}=\langle$ value $\rangle$.
Constraint: $\mathrm{N} \geq \mathrm{M}$.
IFAIL $=20$
SVD failed to converge.

IFAIL $=100$
An internal error has occurred in this routine. Check the routine call and any array sizes. If the call is correct then please contact NAG for assistance.

IFAIL $=-99$
An unexpected error has been triggered by this routine. Please contact NAG.
See Section 3.8 in the Essential Introduction for further information.
IFAIL $=-399$
Your licence key may have expired or may not have been installed correctly.
See Section 3.7 in the Essential Introduction for further information.
IFAIL $=-999$
Dynamic memory allocation failed.
See Section 3.6 in the Essential Introduction for further information.

## $7 \quad$ Accuracy

The calculations are believed to be stable.

## 8 Parallelism and Performance

G03BDF is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

G03BDF 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 reads a loadings matrix and calculates a varimax transformation before calculating $P, R$ and $\sigma$ for a ProMax rotation.

### 10.1 Program Text

```
    Program g03bdfe
    GO3BDF Example Program Text
    Mark 25 Release. NAG Copyright 2014.
    .. Use Statements ..
    Use nag_library, Only: g03baf, g03bdf, nag_wp, x04caf
! .. Implicit None Statement ..
    Implicit None
! .. Parameters ..
    Integer, Parameter :: nin = 5, nout = 6
! .. Local Scalars ..
    Real (Kind=nag_wp) :: acc, g, power
    Integer :: i, ifail, iter, ldfp, ldfs, ldphi, &
                                    ldr, ldro, ldx, lwk, m, maxit, n
    :: stand
    Character (1)
    .. Local Arrays ..
    Real (Kind=nag_wp), Allocatable :: fp(:,:), fs(:,:), phi(:,:), r(:,:), &
                                    ro(:,:), wk(:), x(:,:)
    .. Executable Statements ..
    Write (nout,*) 'GO3BDF Example Program Results'
    Write (nout,*)
    Flush (nout)
! Skip heading in data file
    Read (nin,*)
    Read in problem size
    Read (nin,*) n, m, g, stand, acc, maxit, power
    ldx = n
    ldro = m
    ldfp = n
    ldfs = n
    ldr = m
    ldphi = m
    lwk = 2*n + m*m + 5*(m-1)
    Allocate (fp(ldx,m),x(ldx,m),ro(ldro,m),wk(lwk),phi(ldphi,m),fs(ldfs,m), &
        r(ldr,m))
    Read loadings matrix
    Read (nin,*)(fp(i,1:m),i=1,n)
! Calculate orthogonal rotation
    ifail = 0
    Call g03baf(stand,g,n,m,fp,ldx,x,ro,ldro,acc,maxit,iter,wk,ifail)
```

```
! Calculate ProMax rotation
    ifail = O
    Call g03bdf(stand,n,m,x,ldx,ro,ldro,power,fp,ldfp,r,ldr,phi,ldphi,fs, &
        ldfs,ifail)
    Display results
ifail = 0
Call x04caf('General',' ',n,m,fp,ldfp,'Factor pattern',ifail)
Write (nout,*)
Flush (nout)
ifail = 0
Call x04caf('General',' ',m,m,r,ldr,'ProMax rotation',ifail)
Write (nout,*)
Flush (nout)
ifail = 0
Call x04caf('General',' ',m,m,phi,ldphi,'Inter-factor correlations', &
    ifail)
Write (nout,*)
Flush (nout)
ifail = O
Call x04caf('General',' ',n,m,fs,ldfs,'Factor structure',ifail)
```

End Program g03bdfe

### 10.2 Program Data

GO3BDF Example Program Data
521 'S' 1.OE-5 2003.0 : N,M,G,STAND,ACC,MAXIT,POWER
$0.74215-0.57806$
$0.71370-0.55515$
$0.87899-0.15847$
0.625330 .76621
0.71447 : : End of FP

### 10.3 Program Results



