NAG Library Routine Document

F01RKF

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

F01RKF returns the first ℓ rows of the n by n unitary matrix P^{H}, where P is given as the product of Householder transformation matrices.

This routine is intended for use following F01RJF.

2 Specification

```
SUBROUTINE F01RKF (WHERET, M, N, NROWP, A, LDA, THETA, WORK, IFAIL)

INTEGER                M, N, NROWP, LDA, IFAIL
COMPLEX (KIND=nag_wp) A(LDA,*), THETA(*), WORK(max(M-1,NROWP-M,1))
CHARACTER(1)           WHERET
```

3 Description

P is assumed to be given by

$$P = P_m P_{m-1} \cdots P_1,$$

where

$$P_k = I - \gamma_k u_k u_k^H,$$

$$u_k = \begin{pmatrix} w_k \\ \zeta_k \\ 0 \\ z_k \end{pmatrix}$$

γ_k is a scalar for which $\mathrm{Re}(\gamma_k) = 1.0$, ζ_k is a real scalar, w_k is a $(k-1)$ element vector and z_k is an $(n-m)$ element vector. w_k must be supplied in the kth row of A in elements $\mathrm{A}(k,1),\ldots,\mathrm{A}(k,k-1)$. z_k must be supplied in the kth row of A in elements $\mathrm{A}(k,m+1),\ldots,\mathrm{A}(k,n)$ and θ_k, given by

$$\theta_k = (\zeta_k, \mathrm{Im}(\gamma_k)),$$

must be supplied either in $\mathrm{A}(k,k)$ or in $\mathrm{THETA}(k)$, depending upon the parameter WHERET.

4 References

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

Wilkinson J H (1965) *The Algebraic Eigenvalue Problem* Oxford University Press, Oxford

5 Parameters

1: WHERET – CHARACTER(1) *Input*

On entry: indicates where the elements of θ are to be found.

WHERET = 'I' (In A)

The elements of θ are in A.

WHERET = 'S' (Separate)
The elements of θ are separate from A, in THETA.

Constraint: WHERET = 'I' or 'S'.

2: M – INTEGER *Input*

On entry: m, the number of rows of the matrix A.

Constraint: $\mathrm{M} \geq 0$.

3: N – INTEGER *Input*

On entry: n, the number of columns of the matrix A.

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

4: NROWP – INTEGER *Input*

On entry: ℓ, the required number of rows of P.

If NROWP $= 0$, an immediate return is effected.

Constraint: $0 \leq \mathrm{NROWP} \leq \mathrm{N}$.

5: A(LDA,$*$) – COMPLEX (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array A must be at least $\max(1,\mathrm{N})$.

On entry: the leading m by m strictly lower triangular part of the array A, and the m by $(n-m)$ rectangular part of A with top left-hand corner at element $\mathrm{A}(1,\mathrm{M}+1)$ must contain details of the matrix P. In addition, if WHERET = 'I', the diagonal elements of A must contain the elements of θ.

On exit: the first NROWP rows of the array A are overwritten by the first NROWP rows of the n by n unitary matrix P^{H}.

6: LDA – INTEGER *Input*

On entry: the first dimension of the array A as declared in the (sub)program from which F01RKF is called.

Constraint: $\mathrm{LDA} \geq \max(1,\mathrm{M},\mathrm{NROWP})$.

7: THETA($*$) – COMPLEX (KIND=nag_wp) array *Input*

Note: the dimension of the array THETA must be at least $\max(1,\mathrm{M})$ if WHERET = 'S', and at least 1 otherwise.

On entry: if WHERET = 'S', the array THETA must contain the elements of θ. If $\mathrm{THETA}(k) = 0.0$, P_k is assumed to be I, if $\mathrm{THETA}(k) = \alpha$ and $\mathrm{Re}(\alpha) < 0.0$, P_k is assumed to be of the form

$$P_k = \begin{pmatrix} I & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & I \end{pmatrix},$$

otherwise $\mathrm{THETA}(k)$ is assumed to contain θ_k given by

$$\theta_k = (\zeta_k, \mathrm{Im}(\gamma_k)).$$

If WHERET = 'I', the array THETA is not referenced.

8: WORK(max(M − 1, NROWP − M, 1)) – COMPLEX (KIND=nag_wp) array *Workspace*

9: 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, WHERET $\neq$ 'I' or 'S',
or M < 0,
or N $<$ M,
or NROWP < 0 or NROWP $>$ N,
or LDA $< \max(1, \mathrm{M}, \mathrm{NROWP})$.

7 Accuracy

The computed matrix P satisfies the relation

$$P = Q + E,$$

where Q is an exactly unitary matrix and

$$\|E\| \leq c\epsilon,$$

where ϵ the ***machine precision*** (see X02AJF), c is a modest function of n, and $\|.\|$ denotes the spectral (two) norm. See also Section 7 in F01RJF.

8 Further Comments

The approximate number of floating point operations is given by

$$\frac{8}{3}n[(3n-m)(2\ell-m)-m(\ell-m)], \quad \text{if } \ell \geq m, \text{ and}$$

$$\frac{8}{3}\ell^2(3n-\ell), \quad \text{if } \ell < m.$$

9 Example

This example obtains the 5 by 5 unitary matrix P following the RQ factorization of the 3 by 5 matrix A given by

$$A = \begin{pmatrix} -0.5i & 0.4-0.3i & 0.4 & 0.3-0.4i & 0.3i \\ -0.5-1.5i & 0.9-1.3i & -0.4-0.4i & 0.1-0.7i & 0.3-0.3i \\ -1.0-1.0i & 0.2-1.4i & 1.8 & 0.0 & -2.4i \end{pmatrix}.$$

9.1 Program Text

```
    Program f01rkfe

!     F01RKF Example Program Text

!     Mark 24 Release. NAG Copyright 2012.

!     .. Use Statements ..
      Use nag_library, Only: f01rjf, f01rkf, nag_wp
!     .. Implicit None Statement ..
      Implicit None
!     .. Parameters ..
      Integer, Parameter              :: nin = 5, nout = 6
!     .. Local Scalars ..
      Integer                         :: i, ifail, lda, ldph, m, n, nrowp
!     .. Local Arrays ..
      Complex (Kind=nag_wp), Allocatable :: a(:,:), ph(:,:), theta(:), work(:)
!     .. Intrinsic Procedures ..
      Intrinsic                       :: conjg
!     .. Executable Statements ..
      Write (nout,*) 'F01RKF Example Program Results'
      Write (nout,*)
!     Skip heading in data file
      Read (nin,*)
      Read (nin,*) m, n
      lda = m
      ldph = n
      Allocate (a(lda,n),ph(ldph,n),theta(n),work(n))
      Read (nin,*)(a(i,1:n),i=1,m)
!     ifail: behaviour on error exit
!             =0 for hard exit, =1 for quiet-soft, =-1 for noisy-soft
      ifail = 0
!     Find the RQ factorization of A
      Call f01rjf(m,n,a,lda,theta,ifail)

!     Copy array A into PH and form the n by n matrix conjg(P')
      ph(1:m,1:n) = a(1:m,1:n)
      nrowp = n

      ifail = 0
      Call f01rkf('Separate',m,n,nrowp,ph,ldph,theta,work,ifail)

      Write (nout,*) 'Matrix  P'
      Write (nout,99999)(conjg(ph(1:nrowp,i)),i=1,n)

99999 Format (5(' (',F6.3,',',F6.3,')':))
    End Program f01rkfe
```

9.2 Program Data

```
F01RKF Example Program Data
  3     5                                                                   : m, n
( 0.00,-0.50) ( 0.40,-0.30) ( 0.40, 0.00) ( 0.30, 0.40) ( 0.00, 0.30)
(-0.50,-1.50) ( 0.90,-1.30) (-0.40,-0.40) ( 0.10,-0.70) ( 0.30,-0.30)
(-1.00,-1.00) ( 0.20,-1.40) ( 1.80, 0.00) ( 0.00, 0.00) ( 0.00,-2.40)   : a
```

9.3 Program Results

```
 F01RKF Example Program Results

 Matrix  P
 (-0.197, 0.197) ( 0.164,-0.492) ( 0.277,-0.277) ( 0.364, 0.321) ( 0.012, 0.514)
 ( 0.039, 0.276) (-0.295,-0.426) (-0.055,-0.388) (-0.475, 0.098) (-0.419,-0.299)
 ( 0.315,-0.158) ( 0.452,-0.320) (-0.499,-0.000) (-0.276,-0.305) (-0.034, 0.387)
 ( 0.197,-0.591) (-0.047,-0.331) ( 0.000, 0.000) ( 0.512,-0.047) (-0.361,-0.324)
 (-0.118,-0.565) ( 0.033, 0.208) (-0.000,-0.666) (-0.229, 0.207) ( 0.290, 0.025)
```