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A NUMERICAL ALGORITHM FOR THE CALCULATION OF COEFFICIENTS IN MOVING AVERAGES

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CONTENTS

1. BACKGROUND AND NOTATION FOR THE NUMERICAL ALGORITHM

1.0 General

Given a vector of values $\hat{\lambda} = (\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_m)^T$.

For given integer a construct coefficients r_j, $j = 1, 2, \ldots, 2a+1$, and Y_j^t, $t = 1, 2, \ldots, a$, $j = 1, 2, \ldots, a+t$ in the averaging formulas

$$\lambda_t^* = \sum_{j=1}^{a+t} Y_j^t \hat{\lambda}_j; \quad t = 1, 2, \ldots, a;$$

$$\lambda_t^* = \sum_{j=1}^{2a+1} r_j \hat{\lambda}_{t+j-a-1}; \quad t = a+1, a+2, \ldots, m-a;$$

$$\lambda_{m+1-t}^* = \sum_{j=1}^{a+t} Y_j^t \hat{\lambda}_{m+1-j}; \quad t = a, a-1, \ldots, 1.$$

The coefficients r_j shall be symmetric with respect to r_{a+1}, i.e.,

$r_{a+1+j} = r_{a+1-j}$; $j = 1, 2, \ldots, a$. In Section 1.2 we will use the notation $Y_j^{a+1} = r_j$; $j = 1,2,\ldots, 2a+1$. The coefficients shall be optimal in a certain sense defined in Section 1.1 and satisfy certain constraints defined in Section 1.4.

For a general statistical motivation of this numerical problem and further analysis of the method of moving averages, see Hoem (1978) and Linnemann (1979, 1980).

This paper deals solely with the practical computer implementation of a problem suggested to the present author by Jan M. Hoem.

1.1 Optimization problem

Define for given integer $z > 0$

$$L = \sum_{t=1}^{m-z} (\Delta^z \lambda_t^* - \Delta^z \hat{\lambda}_t)^2,$$

where Δ is the forward difference

$$\Delta\lambda_t = \lambda_{t+1} - \lambda_t$$

and Δ^z denotes z applications of Δ.

The expression for L is a quadratic function in the coefficients r_j, Y_j^t.

If we number the unknown coefficients in the way described in Section 1.2, we can write

$$L = \underline{y}^T Q \, \underline{y}$$

where the matrix Q can be constructed in the sequence of steps described in Appendix 1.

1.2 Numbering of the unknowns

Arrange the unknown coefficients Y_j^t in a table as follows.

j \ t	1	2	3		a
1	Y_1^1	Y_1^2	Y_1^3	...	Y_1^a
2	Y_2^1	Y_2^2	Y_2^3	...	Y_2^a
⋮	⋮				
a+1	Y_{a+1}^1	Y_{a+1}^2	Y_{a+1}^3	...	Y_{a+1}^a
a+2		Y_{a+2}^2	Y_{a+2}^3	...	Y_{a+2}^a
a+3			Y_{a+3}^3	⋱	⋮
⋮					
a+a					Y_{a+a}^a

Then define a vector $\underline{\underline{y}}$ containing the unknowns of this table in lexiographic order, i.e., numbered line by line according to

$$y_{\text{index}} = Y_j^t,$$

with

$$\text{index} = \begin{cases} (j-1)\,a + t; & 1 \leq j \leq a+1; \quad 1 \leq t \leq a; \\ a^2 + a + t - 1; & j = a+2; \quad 2 \leq t \leq a; \\ a^2 + a + a - 1 + t - 2; & j = a+3; \quad 3 \leq t \leq a; \\ \vdots & \\ a^2 + \tfrac{1}{2}a(a-1); & j = a+a; \quad t = a. \end{cases}$$

For example for a = 3 we get the following indexing table.

J		2	3
		2	3
2	4	5	6
3	7	8	9
4	10	11	12
5		13	14
6			15

The unknowns $r_1, r_2, \ldots, r_{a+1}$ are adjoined according to

$$y^2_{a+!(a-1)+j} = r_j ; \quad J \quad 1, 2, \cdots, a+1 .$$

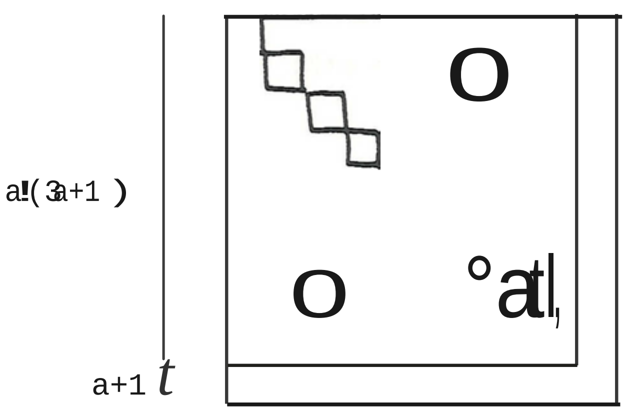
Denote by

$$n = a^2 + ia(a-1) + a + 1$$

the total number of unknowns.

1.3 Data structure for the matrix Q

The matrix Q is symmetric, positive definite and has the following structure of non-zero elements (cf. Appendix 1).



To suit the NAG-routine F01MCF we use the skyline or envelope storage scheme for this matrix. Only half the matrix is needed and only the elements from the first non-zero element of a row to the diagonal element of the same row need to be stored for each row. The data of the matrix is stored in a long vector together with an integer vector that points to the first non-zero element of each row. For further technical details, see the description of the parameters of F01MCF in the NAG library manual.

1.4 Constraints

All the formulas in Section 1.1 shall be exact for polynomials of degree less than d (a given integer), i.e., if

$$\hat{\lambda}_j = P(x_j); \quad j = 1, 2, \ldots, m;$$

with P a polynomial of degree d-1 and $x_j = x_0 + j \cdot \Delta x$, $j=1,2,\ldots, m$ for some given Δx, then

$$\lambda_t^* = P(x_t)$$

for all $t = 1, 2, \ldots, m$.

These conditions can be expressed in several equivalent ways. They all amount to d equations for each of the sets of coefficients

$$\{Y_1^t, Y_2^t, \ldots, Y_{a+x}^t\}; \quad t = 1, 2, \ldots, a+1.$$

In all there are $(a+1)\times d$ equations. Due to the symmetry-condition for r_j, $j = 1, 2, \ldots, 2a+1$; some of the equations for

$$Y_j^{a+1}; \quad j = 1, 2, \ldots, a+1$$

are redundant, see below.

We have chosen to construct sets of orthogonal polynomials

$\{\phi_s^t(x)\}_{s=0}^{d-1}$ for each of the intervals $I_t \equiv [x_1, x_{a+t}]$ $t = 1, 2, \ldots, a+1$ to use as bases for the space of polynomials of degree d-1 on each interval I_t. The polynomials are othogonal with respect to the inner product

$$\langle f,g\rangle_t = \sum_{i=1}^{a+t} f(x_i)\, g(x_i)$$

This special choice of basis is motivated by a wish to get orthogonal rows for the matrix of constraints.

The constraints can be written

$$\sum_{j=1}^{a+t} Y_j^t\, \phi_s^t(x_j) = \phi_s^t(x_t);$$

$$s = 0, 1, \ldots, d-1;$$

$$t = 1, 2, \ldots, a+1;$$

i.e.,

$$V_t \underline{\underline{Y}}^t = \underline{\underline{\Phi}}^t; \quad t = 1, 2, \ldots, a+1;$$

where

$$\underline{\underline{Y}}^t = \begin{bmatrix} Y_1^t \\ Y_2^t \\ \cdot \\ \cdot \\ \cdot \\ Y_{a+1}^t \end{bmatrix};$$

$$\underline{\underline{\Phi}}^t = \begin{bmatrix} \phi_0^t(x_t) \\ \phi_1^t(x_t) \\ \cdot \\ \cdot \\ \cdot \\ \phi_{d-1}^t(x_t) \end{bmatrix};$$

$$V_i = \begin{bmatrix} \phi_0^t(x_1)\ , & \phi_0^t(x_2)\ , & \ldots, \phi_0^t(x_{a+t}) \\ \phi_1^t(x_1)\ , & \phi_1^t(x_2)\ , & \ldots, \phi_1^t(x_{a+t}) \\ \cdot & & \\ \cdot & & \\ \cdot & & \\ \phi_{d-1}^t(x_1), & \phi_{d-1}^t(x_2) & \ldots\ \phi_{d-1}^t(x_{a+t}) \end{bmatrix} .$$

These are a+1 uncoupled sets of equations.

For t = a+1 the symmetry condition reduces the equations to

$V_0\underline{\underline{r}} = \underline{\underline{\Phi}}^{a+1}$

with

$$\underline{\underline{r}} = \begin{bmatrix} r_1 \\ r_2 \\ \cdot \\ \cdot \\ \cdot \\ r_{a+1} \end{bmatrix} ;$$

$$V_0 = \begin{bmatrix} \phi_0^{a+1}(x_1) + \phi_0^{a+1}(x_{2a+1})\ , & \phi_0^{a+1}(x_2) + \phi_0^{a+1}(x_{2a}), & \ldots, \phi_0^{a+1}(x_{a+1}) \\ \phi_1^{a+1}(x_1) + \phi_1^{a+1}(x_{2a+1})\ , & \phi_1^{a+1}(x_2) + \phi_1^{a+1}(x_{2a}), & \ldots, \phi_1^{a+1}(x_{a+1}) \\ \cdot & & \\ \cdot & & \\ \cdot & & \\ \phi_{d-1}^{a+1}(x_1) + \phi_{d-1}^{a+1}(x_{2a+1})\ , & \phi_{d-1}^{a+1}(x_2) + \phi_{d-1}^{a+1}(x_{2a}), & \ldots, \phi_{d-1}^{a+1}(x_{a+1}) \end{bmatrix} .$$

V_0 is obtained by folding V_{a+1} along column a+1 and adding columns.

Due to the fact that the points x_1, $x_2, \ldots,$ x_{2a+1} are symmetric around x_{a+1}, the rows containing odd numbered polynomials ϕ_i^{a+1}, i=1,3,... are identically zero, also these right hand sides are identically zero. Thus, these equations read 0=0 and can be omitted.

The remaining equations are written

$$V^*\underline{\underline{r}} = \underline{\underline{\phi}}^*$$

with

$$\underline{\underline{r}} = \begin{bmatrix} r_1 \\ r_2 \\ \cdot \\ \cdot \\ \cdot \\ r_{a+1} \end{bmatrix} ;$$

$$\underline{\underline{\phi}}^* = \begin{bmatrix} \phi_0^{a+1}(x_{a+1}) \\ \phi_2^{a+1}(x_{a+1}) \\ \vdots \\ \phi_{2p}^{a+1}(x_{a+1}) \end{bmatrix} ;$$

$$V^* = \begin{bmatrix} \phi_0^{a+1}(x_1) + \phi_0^{a+1}(x_{2a+1}) \,,\; \phi_0^{a+1}(x_2) + \phi_0^{a+1}(x_{2a}),\ldots,\; \phi_0^{a+1}(x_{a+1}) \\ \phi_2^{a+1}(x_1) + \phi_2^{a+1}(x_{2a+1}) \,,\; \phi_2^{a+1}(x_2) + \phi_2^{a+1}(x_{2a}),\ldots,\; \phi_2^{a+1}(x_{a+1}) \\ \cdot \\ \cdot \\ \cdot \\ \phi_{2p}^{a+1}(x_1) + \phi_{2p}^{a+1}(x_{2a+1}) \,,\; \phi_{2p}^{a+1}(x_2) + \phi_{2p}^{a+1}(x_{2a}),\ldots,\; \phi_{2p}^{a+1}(x_{a+1}) \end{bmatrix} ;$$

where p is the integer part of $\frac{d-1}{2}$.

The number of constraint equations is

$$n_c = a \cdot d + p + 1.$$

Note: Even if another base is used to construct the constraint equations, the same redundancy is obtained, maybe in disguise, such that there are only p+1 independent equations for r_1, r_2,..., r_{a+1}. If the redundant equations are not removed, the algorithm will break down.

All the equations can be summarized as

$$V\underline{\underline{y}} \equiv \underline{\underline{v}},$$

where V is an $n_c \times n$ sparse matrix with special structure and

$$\underline{\underline{v}} = \begin{bmatrix} \underline{\underline{\Phi}}^1 \\ \underline{\underline{\Phi}}^2 \\ \cdot \\ \cdot \\ \cdot \\ \underline{\underline{\Phi}}^a \\ \underline{\underline{\Phi}}^* \end{bmatrix} .$$

1.5 Data structure for the constraints

We store the matrices V* and V_t, $t = 1, 2, \ldots, a$, in a rectangular matrix VT in the following fashion. For our description denote the transpose of VT by U. Then

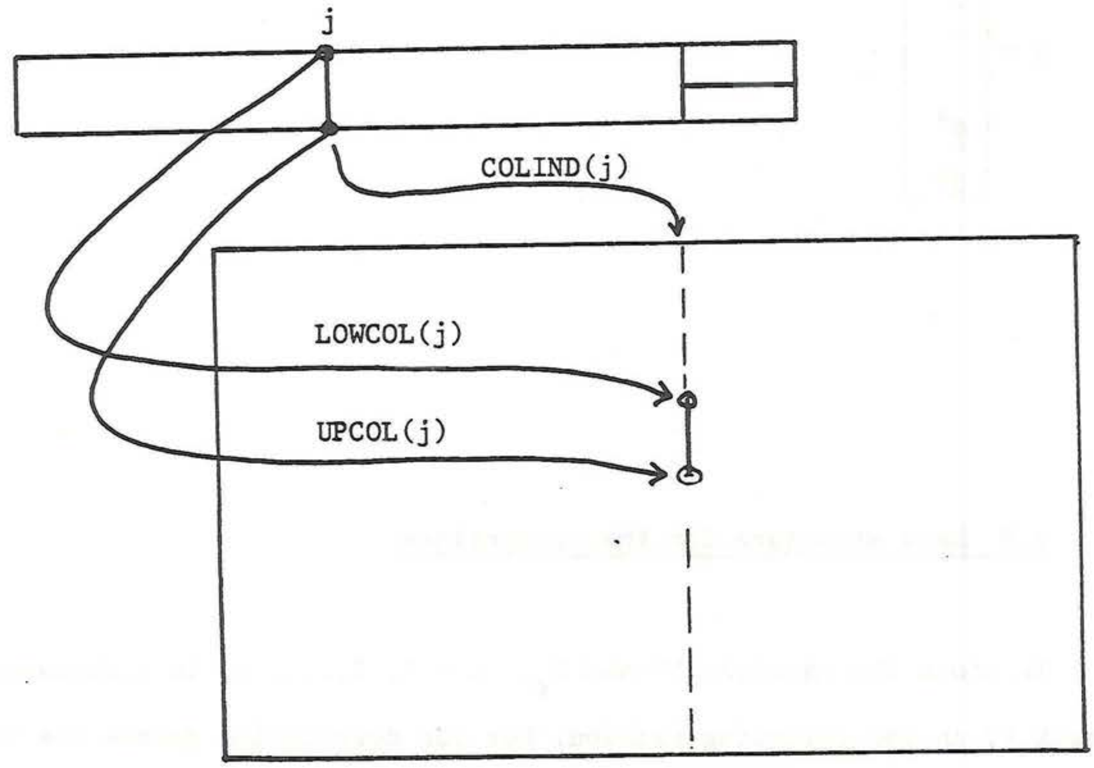
$$U = \begin{array}{|c|c|c|c|c|c|} \hline V_1 & V_2 & V_3 & \cdots & V_a & \begin{array}{c} V^* \\ \hline 0 \end{array} \\ \hline \end{array}$$

Together with VT we store six integer vectors that carry information on the structure of the $n_c \times n$ matrix V of constraints

$$V\underline{\underline{y}} = \underline{\underline{v}}.$$

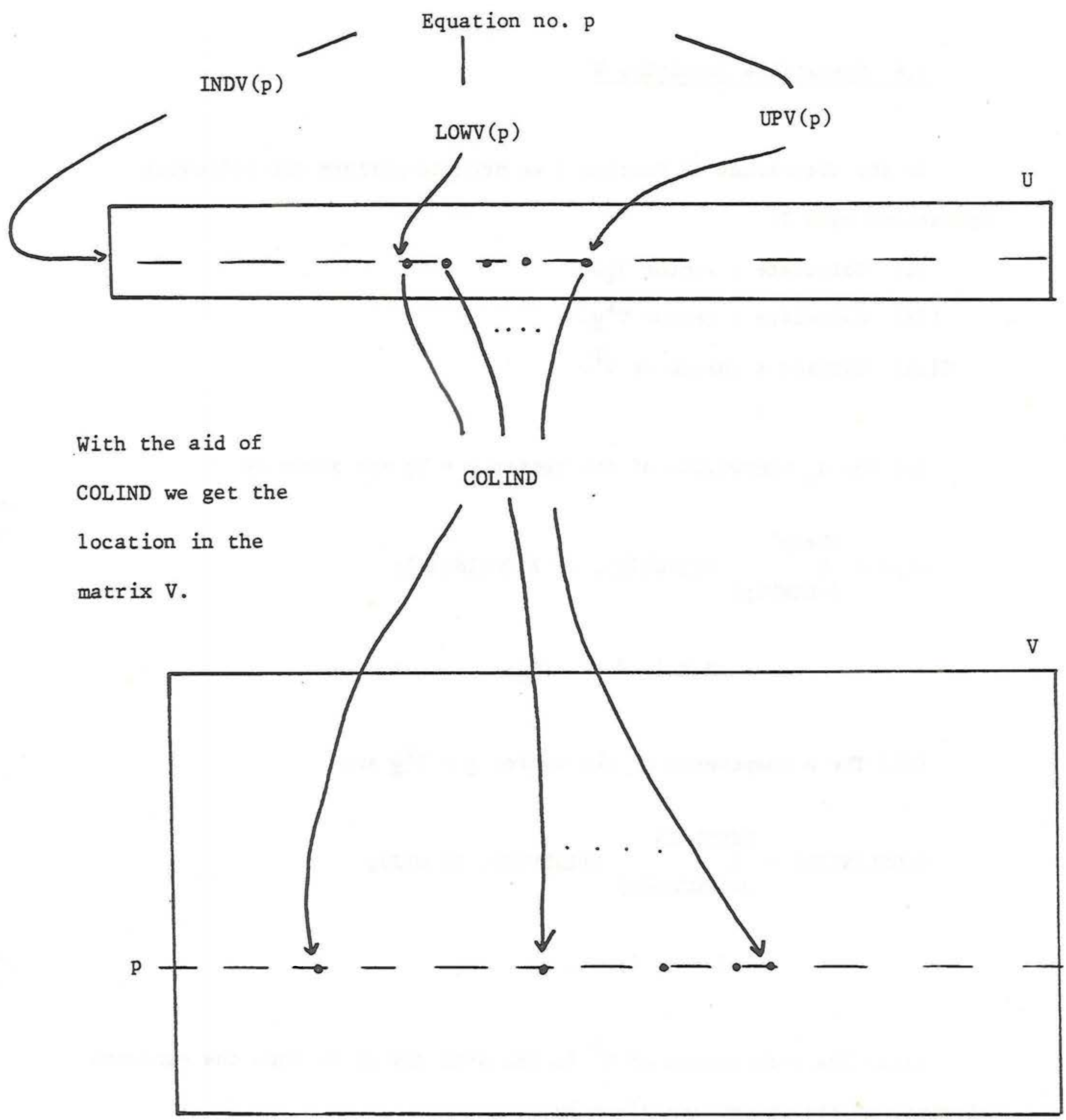
For each of the n columns of U the components of the vector COLIND tell the index of the corresponding unknown in $\underline{\underline{y}}$, i.e., the column number of the corresponding column in the matrix V.

The vectors LOWCOL and UPCOL tell for each column of U the lower row-index and upper rowindex for that column's location in V.



For most of the columns UPCOL(j) - LOWCOL(j) = d, but for the last a+1 columns of U the difference is smaller.

There are n_c rows in V, for each row the vectors INDV, LOWV, UPV indicate the location in the matrix U of the coefficients for the actual row. INDV gives the row number, LOWV and UPV the lower columnindex and the upper columnindex respectively.



INDV(p) takes values in the set $\{1, \ldots, d\}$.

1.6 Operations involving V

In the algorithms of Section 2 we need to perform the following operations with V:

(i) Calculate a vector $V\underline{\underline{z}}$.

(ii) Calculate a vector $V^T\underline{\underline{w}}$.

(iii) Extract a column of V^T.

(i) The n_c components of the vector $\underline{\underline{w}} = V\underline{\underline{z}}$ are given by

$$w(p) = \sum_{j=LOWV(p)}^{UPV(p)} U(INDV(p),\ J)\ Z(COLIN(J));$$

$$p = 1,\ 2, \ldots,\ n_c.$$

(ii) The n components of the vector $\underline{\underline{z}} = V^T\underline{\underline{w}}$ are

$$Z(COLIN(I)) = \sum_{J=LOWCOL(I)}^{UPCOL(I)} U(INDV(J),\ I)\ w(J);$$

$$I = 1,\ 2, \ldots,\ n.$$

(iii) The p-th column of V^T is the p-th row of V. Thus the non-zero elements of the column are given by

$$Z(COLIN(J)) = U(INDV(p),\ J);$$

$$J = LOW(P),\ LOWV(p) + 1, \ldots,\ UPV(p).$$

In the program we have used the matrix $VT = U^T$ instead of U so whenever the matrix element U(p,q) appears above we should replace it with VT(q,p).

2. NUMERICAL SOLUTION

2.1 Basic Problem

The problem

$$\begin{cases} \min\limits_{\underline{y}} \tfrac{1}{2}\underline{y}^T Q \underline{y} \\ \text{for} \\ V\underline{y} = \underline{v}, \end{cases}$$

with Q an $n \times n$ symmetric positive definite matrix,

V an $n_c \times n$ matrix,

$\underline{y}$ an n-vector, and

$\underline{v}$ an n_c-vector, $n_c \ll n$,

has the solution

$$\underline{y} = Q^{-1}V^T(VQ^{-1}V^T)^{-1}\underline{v}.$$

See e.g. Gill et al. (1981, Section 5.4.1) and Section 2.2 of this paper.

2.1.1 Algorithm

The solution is computed in the following sequence of steps, using subroutines from the NAG-library.

1. Compute the Choleski factorization R^TR of Q. Here R is an upper triangular $n \times n$-matrix. Due to the special structure of Q this is best done by the NAG-routine F01MCF.

2. Define $Z = Q^{-1}V^T$. Z is an $n \times n_c$-matrix. The n_c columns of Z are the solutions of the n_c systems of linear equations

$$QZ = V^T.$$

These systems are solved using the Choleski factorization of Q. This is done by the NAG-routine F04MCF.

3. Form the symmetric, positive definite matrix

$$H = VQ^{-1}V^T = VZ.$$

H is a $n_c \times n_c$-matrix. Only the upper triangular part of H need to be computed.

4. Define $\underline{\underline{w}} = H^{-1}\underline{\underline{v}}$. The n_c-vector $\underline{\underline{w}}$ is the solution of the symmetric "small" linear system

$$H\underline{\underline{w}} = \underline{\underline{v}}$$

which is solved by the NAG-routine F04ASF.

5. Form $\underline{\underline{u}} = V^T\underline{\underline{w}}$. $\underline{\underline{u}}$ is an n-vector.

6. Finally compute $\underline{\underline{y}} = Q^{-1}\underline{\underline{u}}$. This is equivalent to solving the system of linear ewuations

$$Q\underline{\underline{y}} = \underline{\underline{u}},$$

which is done by F04MCF.

Note that this algorithm never explicitly computes the inverses of Q and H. The inverses have no structure even if Q and H have, so they should be avoided. The Choleski-factors, however, have the same kind of structure as the original matrices. For numerical calculations it is always advisable to avoid explicit inverses unless you are interested in the individual elements of them. In our algorithm we are only interested in operating with the inverse on certain given vectors.

2.2 Modified problem, some values of $\underline{\underline{y}}$ given

The problem

$$\begin{cases} \min\limits_{\underline{\underline{y}}} \frac{1}{2}\underline{\underline{y}}^T Q\underline{\underline{y}} \\ \text{for} \\ V\underline{\underline{y}} = \underline{\underline{v}}, \\ y_i = c_i, \quad i = n-a, n-a+1, \dots, n, \end{cases}$$

can be solved by first enlarging the set of constraints $V\underline{\underline{y}} = \underline{\underline{v}}$ with the k constraints $y_i = c_i$ to

$$W\underline{\underline{y}} = \underline{\underline{w}},$$

with W an $(n_c + k)\times n$ matrix and $\underline{\underline{w}}$ an $(n_c + k)$ vector. Then the problem is solved as in Section 2.1. This, however, may be grossly inefficient.

The following transformations give a much simpler problem.

The idea is to eliminate y_i, $i = n-a,\ldots, n$, from both the quadratic form and the constraints.

Introduce the following notation

$$\underline{\underline{y}} = \begin{bmatrix} \underline{\underline{x}} \\ \underline{\underline{r}} \end{bmatrix} \begin{array}{l} \text{(n-a-1 components)} \\ \text{(a+1 components).} \end{array}$$

Let $k = a+1$.

Partition Q as follows (the same partition as in Appendix 1):

$$\begin{array}{cc} Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{12}^T & Q_{22} \end{bmatrix} & \begin{array}{l} (n-k) \\ (k) \end{array} \\ \quad\;\; (n-k) \quad (k) & \end{array},$$

and V as

$$\begin{array}{c} V = [V_A \quad V_B]. \\ \quad\;\; (n-k) \;\; (k) \end{array}$$

The quadratic form is then

$$\underline{\underline{y}}^T Q \underline{\underline{y}} = (\underline{\underline{x}}^T \underline{\underline{r}}^T) \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{12}^T & Q_{22} \end{bmatrix} \begin{bmatrix} \underline{\underline{x}} \\ \underline{\underline{r}} \end{bmatrix}$$

$$= \underline{\underline{x}}^T Q_{11} \underline{\underline{x}} + 2\underline{\underline{x}}^T \underline{\underline{b}} + \alpha$$

with

$$\underline{\underline{b}} = Q_{12}\underline{\underline{r}} \quad \text{and} \quad \alpha = \underline{\underline{r}}^T Q_{22}\underline{\underline{r}}.$$

The constraints become

$$V\underline{\underline{y}} = \begin{bmatrix} V_A & V_B \end{bmatrix} \begin{bmatrix} \underline{\underline{x}} \\ \underline{\underline{r}} \end{bmatrix} = V_A\underline{\underline{x}} + V_B\underline{\underline{r}} = \underline{\underline{v}},$$

i.e., $$V_A\underline{\underline{x}} = \underline{\underline{v}} - V_B\underline{\underline{r}} .$$

Due to the special form of V (cf. Sec. 1.4 - 1.5) this is equivalent to

$$W\underline{\underline{x}} \equiv \underline{\underline{m}},$$

where w is an $n_w \times (n-k)$ matrix consisting of the first n_w rows and $(n-k)$ first columns of V, $\underline{\underline{m}}$ consists of the n_w first components of $\underline{\underline{v}}$, and $n_w = a \cdot d$. Thus we have dropped the constraints on $\underline{\underline{r}}$ and incorporated the known values of $\underline{\underline{r}}$ into the linear and constant terms of the quadratic form.

Our problem is now

$$\begin{cases} \min\limits_{\underline{\underline{x}}} \ \tfrac{1}{2}\underline{\underline{x}}^T Q_{11}\underline{\underline{x}} + \underline{\underline{x}}^T\underline{\underline{b}} + \tfrac{1}{2}\alpha \\ \text{for} \\ W\underline{\underline{x}} = \underline{\underline{m}} . \end{cases}$$

The solution is obtained from the unconstrained problem ($\underline{\underline{\lambda}}$ is a vector of Lagrange multipliers)

$$\min_{\underline{\underline{x}},\underline{\underline{\lambda}}} \tfrac{1}{2}\underline{\underline{x}}^T Q_{11}\underline{\underline{x}} + \underline{\underline{x}}^T\underline{\underline{b}} + \tfrac{1}{2}\alpha - (W\underline{\underline{x}}-\underline{\underline{m}})^T\underline{\underline{\lambda}} \equiv \psi(\underline{\underline{x}};\underline{\underline{\lambda}}).$$

The solution is given by the condition

$$\text{grad}_{\underline{\underline{x}},\underline{\underline{\lambda}}}\psi = 0,$$

i.e.

$$\begin{cases} Q_{11}\underline{\underline{x}} + \underline{\underline{b}} - W^T\underline{\underline{\lambda}} = 0, \\ W\underline{\underline{x}} - \underline{\underline{m}} = 0. \end{cases}$$

In partitioned form we write

$$\begin{bmatrix} Q_{11} & -W^T \\ W & 0 \end{bmatrix} \begin{bmatrix} \underline{\underline{x}} \\ \underline{\underline{\lambda}} \end{bmatrix} = \begin{bmatrix} -\underline{\underline{b}} \\ \underline{\underline{m}} \end{bmatrix} .$$

Multiply the first partition with WQ_{11}^{-1} and subtract from the second partition.

This gives

$$\begin{bmatrix} Q_{11} & -W^T \\ 0 & WQ_{11}^{-1}W^T \end{bmatrix} \begin{bmatrix} \underline{\underline{x}} \\ \underline{\underline{\lambda}} \end{bmatrix} = \begin{bmatrix} -\underline{\underline{b}} \\ \underline{\underline{m}} + WQ_{11}^{-1}\underline{\underline{b}} \end{bmatrix} ,$$

i.e.

$$\underline{\underline{\lambda}} = (WQ_{11}^{-1}W^T)^{-1}(\underline{\underline{m}} + WQ_{11}^{-1}\underline{\underline{b}}).$$

Insert this into the first partition and solve for $\underline{\underline{x}}$ to get

$$\underline{\underline{x}} = Q_{11}^{-1}\ [-\underline{\underline{b}} + W^T\underline{\underline{\lambda}}]$$

$$= Q_{11}^{-1}\ [-\underline{\underline{b}} + W^T(WQ_{11}^{-1}W^T)^{-1}(\underline{\underline{m}} + WQ_{11}^{-1}\underline{\underline{b}}].$$

Note that for $\underline{\underline{b}} = 0$ we get the same expression as in Section 2.1.

2.2.1 Algorithm

The solution is computed in the following sequence of steps, using subroutines from the NAG-library. The only differences compared to the algorithm of Section 2.1.1 are the steps 0, 1b, 1c and 5b.

0. Compute $\underline{\underline{b}} = Q_{12}\underline{\underline{r}}$.

1a. Compute the Choleski factorization R^TR of Q_{11}. R is an upper triangular n×n-matrix. Due to the special structure of Q_{11}, this is best done by the NAG-routine F01MCF.

1b. Solve $Q_{11}\underline{\underline{t}} = \underline{\underline{b}}$.

1c. Put $\underline{\underline{\tilde{m}}} = \underline{\underline{m}} + W\underline{\underline{t}}$.

2. Define $Z = Q_{11}^{-1}V_1^T$. Z is an $n \times n_c$ matrix. The n_c columns of Z are the solutions of the n_c systems of linear equations

$$Q_{11}Z = V_1^T.$$

These systems are solved using the Choleski factorization of Q. This is done by the NAG-routine F04MCF.

3. Form the symmetric, positive definte matrix

$$H = V_1Q_{11}^{-1}V_1^T = V_1Z.$$

H is an $n_c \times n_c$ matrix. Only the upper triangular part of H needs to be computed.

4. Define $\underline{\underline{w}} = H^{-1}\underline{\underline{m}}$. The n_c-vector $\underline{\underline{w}}$ is the solution of the symmetric "small" linear system

$$H\underline{\underline{w}} = \underline{\underline{m}},$$

which is solved by the NAG-routine F04ASF.

5a. Form $\underline{\underline{u}} = V_1^T\underline{\underline{w}}$. $\underline{\underline{u}}$ is an n-vector.

5b. Put $\underline{\underline{\tilde{u}}} = -\underline{\underline{b}} + \underline{\underline{u}}$.

6. Finally, compute $\underline{\underline{y}} = Q_{11}^{-1}\underline{\underline{u}}$. This is equivalent to solving the system of linear equations

$$Q_{11}\underline{\underline{y}} = \underline{\underline{u}},$$

which is done by F04MCF.

3. USER INSTRUCTION

This instruction is for the installation on the VAX-computer in the Physics Department of the University of Stockholm.

The data to the program are presented via a terminal in an interactive session in one of the following types. The sessions are hopefully self-explained. Underlined items are the user's replies to the computer.

3.1 No coefficients specified

The program is started by the first command.

```
  run glid
The no.of points in the main moving average is 2*a+1.
(1<=a<=40)
 Give tail length a:
3
T°he graduation method will be exact for polynomials of
degree G (<=5 and <=a).
 Give G:
i.
The object function contains a difference of order z.
 (1 <=z<=5 and z<a )
 Give z:
1
The no. of observations is m (>2*a+z).
 Give m:
22.
Coefficients of the main moving average known?(YES/NO)
.B2.
For results, see file FRI2107.50
```

The results from the calculation are stored in an automatically generated file with the name

FRI<G><Z><2a+1>.<m>

where < > means the character of the numerical value of the enclosed quantity.

The session above generated the result

95681	31121	982	-7533
12956	27224	21356	9656
-12956	31605	39794	29177
4319	30636	42668	37401
0	-20586	4951	29177
0	0	-9751	9656
0	0	0	-7533

TRACE= 0.903714E+01

The table contains the unknowns Y_j^t, $j = 1, 2, \ldots, a+1$, $t = 1, 2, \ldots, a+1$, arranged in the way described in Section 1.2, i.e., the first column contains $Y_1^1, Y_2^1, \ldots, Y_4^1$ and the last column contains $r_1, r_2, \ldots, r_7$. Also TRACE $= \Sigma Q_i$.

3.2 The coefficients of the main moving average specified

In this case a file containing the coefficients r_j, $j = 1, 2, \ldots, a+1$, of the main moving average must be prepared before the program is executed.

In the file the coefficients must be stored as
r<1>
r<2>

r<a+1>
i.e., sequentially with one value on each row.
The numbers must contain a decimal point, 1.e., even if the value is 5500 it must be given as 5500.0.
If r<a+l> is greater than 1 the program assumes that the coefficients in the file are scaled by the factor 10**I,where I is a positive integer. In that case the file should be terminated with one row containing the integer I.

Example RC.DAT contains

```
-7533-0
9656.0
29177.0
37401.0
5
```

A session is started with the first command below.

```
run glid
The no. of points in the main moving average is 2*a+1 .
(1<=a<=40)
 Give tail length a:
/..
The graduation method will be exact for polynomials of
degree G (<=5 and <=a).
 Give G:
2
The object function contains a difference of order z.
 (1 <=z<=5 and z<a )
 Give z:
1
The no. of observations is m (>2*a+z).
 Give m:
50
Coefficients of the main moving average known?(YES/NO)

Give the name of the file of the r-coefficients:
rc!'.dat
For results, see file FST2107.KFF
```

The results are again stored in an automatically generated file with the name

FST<G><Z><2a+1>.KFF

The session above generated the result

95681	31121	982	-7533
12956	27224	21355	9656
-12956	31605	39794	29177
4319	30636	42668	37401
0	-20586	4951	29177
0	0	-9751	9656
0	0	0	-7533

with the same organization as in Section 3.1.

4. INSTRUCTIONS FOR INSTALLATION AND MODIFICATION

As the program uses several NAG-library routines, the source files for the main program and all the subroutines should be compiled, linked and loaded together with the appropriate routines from the NAG-library, into an executable module. On the VAX we have named this module GLID.

The program is written in FORTRAN 77, but mast of the program 1s 1n accordance with the rules of standard FORTRAN.

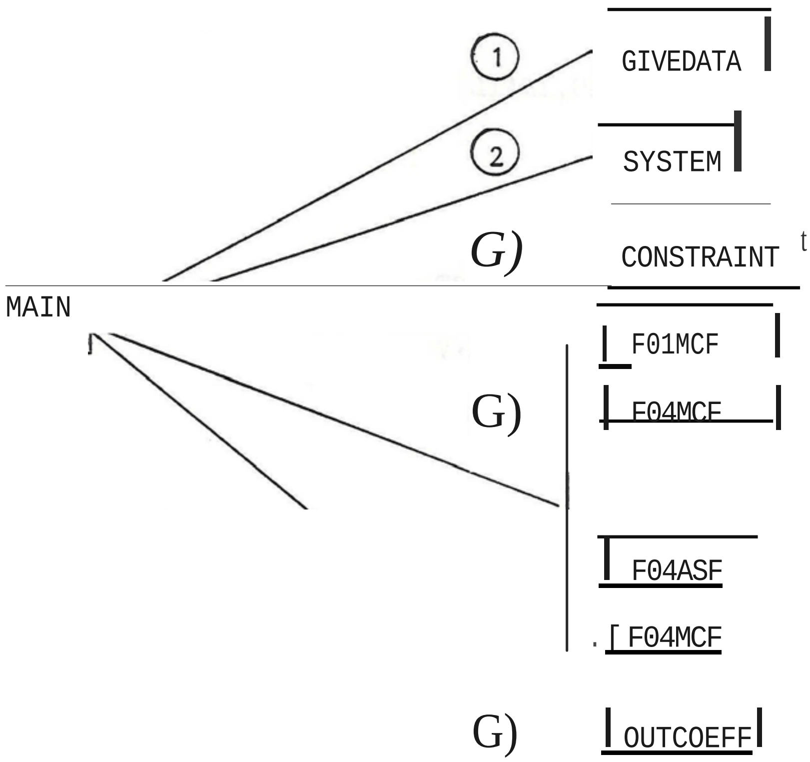
Only the input routine GIVEDATA and the output routine OUTCOEFF use non-standard FORTRAN. In these ·routines the character handling facilities of FORTRAN 77 are used. Furthermore, same system dependent file handling 1s performed ere.

If the program is installed on other systems, these two routines may have to be changed.

5. PROGRAM ORGANIZATION AND LISTING

5.1 The main program

The main modules of the program interact as follows.



The logical variable GIVENR is used to select between the two algorithm paths described in Sections 2.1.1 and 2.2.1.

The following three pages contain a listing of the main program.

```
      REAL*8 VT(2461,6),Z(2461,1),A(128000),DIAG(2461),H(246,246)
      REAL*8 SUM,R(11),WK1(246),WK2(246),Y(246),B(2461),QSUM,V(246)
      INTEGER ND,NA,NZ,M,LOWV (246),UPV(246),INDV (246),COLIN(2461 )
      INTEGER NROW(2461),UP,LOWCOL(2461),UPCOL(2461)
      LOGICAL GIVENR

      CALL GIVEDATA(NA,ND,NZ,M,R,GIVENR)

      CALL SYSTEM(A,NROW,NA,NZ,M,LAL,NOEKV,GIVENR,R,B)

      CALL CONSTRAINT(VT,V,ND,NA,NCON,LOWV,UPV,INDV,LOWCOL,UPCOL,
     * COLIN,GIVENR)

      CALL F01MCF(NOEKV,A,LAL,NROW,A,DIAG,IFAIL)
      IF (IFAIL.NE.0) WRITE(5,91) IFAIL
91    FORMAT('IFAIL=',I5, 'IN F01MCF')

      IF(.NOT.GIVENR) GOTO 190

C        IF THE R-COEFFICIENTS ARE GIVEN WE SOLVE
C              Q<1,1>Z=B     (Q<1,1> IS THE UPPER LEFT PARTITION OF Q)
C        FOLLOWED BY CALCULATION OF V=(VT)**T*Z+V

         DO 110 J=1,NOEKV
            Z(J,1)=B(J)
110      CONTINUE

         NZDIM=2461
         ISELECT=1
         NR=1

         CALL F04MCF(NOEKV,A,LAL,DIAG,NROW,NR,Z,NZDIM,ISELECT,Z,
     C                     NZDIM,IFAIL)


         DO 160 IV=1,NCON
            SUM=0.0
            INDEX=INDV(IV)
            LOW=LOWV (IV)
            UP=UPV(IV)
            DO 150 J=LOW,UP SUM=SUM+VT
               (J,INDEX)*Z(COLIN(J),1)
150         CONTINUE

            V(IV)=SUM+V(IV)
160      CONTINUE

190   CONTINUE

C           CONSTRUCTION OF PROJECTED MATRIX   H=(VT)**T*Q**(-1)*VT

      DO 500 IZ=1,NCON
         DO 200 J=1,NOEKV
            Z(J,1)=0.0
200      CONTINUE
```

```
      INDEX=INDV(IZ)
      LOW=LOWV(IZ)
      UP=UPV(IZ)
      DO 300 J=LOW,UP
         Z(COLIN(J),1)=VT(J,INDEX)
300   CONTINUE

      NZDIM=2461
      ISELECT=1
      NR=1


      CALL F04MCF(NOEKV,A,LAL,DIAG,NROW,NR,Z,NZDIM,ISELECT,Z,
     *                  NZDIM,IFAIL)

      IF (IFAIL.NE.0) WRITE(5,311) IFAIL
311   FORMAT('IFAIL I F04MCF= ',I5)

      DO 400 IV=IZ,NCON
         SUM=0.0
         INDEX=INDV(IV)
         LOW=LOWV(IV)
         UP=UPV(IV)
         DO 390 J=LOW,UP
            SUM=SUM+VT(J,INDEX)*Z(COLIN(J),1)
390      CONTINUE

         H(IZ,IV)=SUM
400   CONTINUE
500 CONTINUE

C    SOLVE H*Y=V

    NHDIM=246

    CALL F04ASF(H,NHDIM,V,NCON,Y,WK1,WK2,IFAIL)

    IF (IFAIL.NE.0) WRITE(5,591) IFAIL
591 FORMAT('IFAIL= ',I5 'I F04ASF ')

C   COMPUTE THE VALUE OF THE QUADRATIC FORM

    QSUM=0
    DO 600 I=1,NCON
       QSUM=QSUM+V(I)*Y(I)
600 CONTINUE

C   FORM THE VECTOR Z=VT*Y

    DO 1500 I=1,NOEKV
       LOW=LOWCOL(I)
       UP=UPCOL(I)
       SUM=0
       DO 1400 J=LOW,UP
          INDEX=INDV(J)
          SUM=SUM+VT(I,INDEX)*Y(J)
1400      CONTINUE
       Z(COLIN(I),1)=SUM
1500   CONTINUE
```

```
      IF (.NOT.GIVENR) GOTO 1560
C       IF THE R-COEFFICIENTS ARE GIVEN WE CALCULATE Z=Z-B
        DO 1550 I=1,NOEKV
          Z(I,1)=Z(I,1)-B(I)
1550      CONTINUE
1560    CONTINUE
C     SOLVE Q*Z=Z
      ISELECT=1
      NZDIM=2461
      NR=1
      CALL F04MCF (NOEKV,A,LAL,DIAG,NROW,NR,Z,NZDIM,ISELECT,Z,NZDIM,IFAIL)
      IF (IFAIL.NE.O) WRITE(5,1591)IFAIL
1591    FORMAT('IFAIL= ,I5, 'I ANROP 2 AV F04MCF )
      IF (.NOT.GIVENR) GOTO 1800
C       WHEN THE R-COEFFICIENTS ARE GIVEN CONCATENATE THOSE TO THE
C       SOLUTIONVECTOR BEFORE PRINTING.
        ILOW=NOEKV+1
        NOTOT=NOEKV+NA+1
        DO 1700 I=ILOW,NOTOT
          Z(I,1)=R(I-NOEKV)
1700      CONTINUE
1800    CONTINUE
      CALL OUTCOEF(Z,QSUM,NA,ND,NZ,M,LOWV,UPV,COLIN,GIVENR)
      END
```

52 The subroutine SYSTEM

The subroutine SYSTEM and the subprograms it uses are listed below.

```
      SUBROUTINE SYSTEM(A,NROW,NA,NZ,M,LAL,NOEKV,GIVENR,RCOEF,B)
      REAL*8 A(1),B(1),RCOEF(1),SL
      INTEGER NROW(1 ),NA,NZ,LAL,NOEKV,M
      INTEGER T(40,40),Q21(41,2420),Q22(41,41),ROWNO,ROWT,COLINDEX
      LOGICAL GIVENR

      CALL TMATRIX(T,NA,NZ )
      CALL QMAT21 (Q21 ,NA,NZ )
      CALL  QMAT22(Q22,NA,NZ,M)

C     STORE THE MATRIX Q IN THE VECTOR A ACCORDING TO THE
C     STORAGE SCHEME FOR THE NAG-ROUTINE F01 .

      NEXTirrnEX=1

C     TREAT THE FIRST NA+1 DIAGONAL BLOCKS OF Q<1,1>

      NA1 =NA+1
      DO 500 IP=1,NA1
         LOW=(IP-1 )*NA
         00 400 I=1,NA
            NSUB=NZ+1
            IF (I.LE.NZ)NSUB=I
            NROW(LOW+I)=NSUB
            JLOW=I-NSUB+1
            DO 300 J=JLOW,I
             A (NEXTINDEX)=2*DFLOAT (T(I,J))
             NEXTINDEX=NEXTINDEX+1
300         CONTINUE
400      CONTINUE
500   CONTINUE

C     CONTINUE WITH THE DIAGONAL BLOCKS NA+2,NA+3, ••• 2*NA OF Q<1,1>

      ROWNO=NA
      NA2=NA+2
      NTW0=2*NA
      DO 1500 IP=NA2,NTWO
         LOW=LOW+ROWNO
         ROWNO=ROWN0-1
         ROWT=IP-NA
         DO 1400 I=1,ROWNO
            NSUB=NZ+1
            IF (ROWT.LE.NZ)NSUB=ROWT
            JLOW=ROWT-NSUB+1
            IF (JLOW.LT.(IP-NA))JLOW=IP-NA
            NROW (LOW+I)=ROWT-JLOW+1
            DO 1300 J=JLOW,ROWT
```

```
            A (NEXTINDEX)=2*DFLOAT (T(ROWT,J))
            NEXTINDEX=NEXTINDEX +1
1300            CONTINUE
         ROWT=ROWT+1
1400          CONTINUE

1500       CONTINUE

C    REMEMBER THE NUMBER OF STORED ELEMENTS OF Q<1,1>

      KLAL=NEXTINDEX-1

C    DECODING OF Q21 AND Q22

      NOROW=NA+1
      NCOL=NA*(3*NA+1 )/2
      DO 2500 I=1,NOROW
         COLINDEX= 1
         DO 2100 J=1,NCOL
            IF (Q21(I,J).NE.O) GOTO 2101
            COLINDEX=COLINDEX+1
2100          CONTINUE
2101          CONTINUE
         NROW(NCOL+I )=NCOL+1 -COLINDEX+I
         IF (COLINDEX.GT.NCOL) GOTO 2201
         DO 2200 J=COLINDEX,NCOL
            A(NEXTINDEX)=DFLOAT(Q21(I,J))
            NEXTINDEX=NEXTINDEX+1
2200          CONTINUE
2201          CONTINUE

         DO 2300 J=1,I
            A(NEXTINDEX)=DFLOAT (Q22(I,J))
            NEXTINDEX=NEXTINDEX+1
2300          CONTINUE

2500       CONTINUE

      LAL=NEXTINDEX-1
      NOEKV= NCOL+NOROW

      IF (.NOT.GIVENR) GOTO 3500

C    IF THE R-COEFFICIENTS ARE GIVEN THE SIZE OF THE MATRIX IS
C    REDUCED AND THE VECTOR   B=Q<1,2>R IS CALCULATED.
      LAL=KLAL
      NOEKV=NOEKV- (NA+1 )
      NA1 =NA+1
      IUP=NA*(3*NA+1 )/2
      DO 3000 I=1,IUP
         SL=O
         DO 2900 J=1 ,NA1
            SL=SL+Q21(J,I)*RCOEF(J)
2900          CONTINUE
         B(I)=SL
3000       CONTINUE

3500       CONTINUE

      RETURN
      END
```

```
      SUBROUTINE QMAT22(Q22,NA,NZ,M)
      INTEGER Q22(41,1),S1(81,81),S2(81,81),K22(81,81),PZ(41),Q,QUP
      INTEGER QLOW,NA,NZ,M

      CALL FACTZ(NZ,PZ)

      IUP=2*NA+1-NZ
      DO 500 IP=1,IUP
         IPOS=1
         QUP=NZ-1
         DO 400 Q=0,QUP
            ISUM=0
            JUP=NZ-Q
            DO 300 J=1,JUP
            ISUM=ISUM+J*PZ(J)*PZ(J+Q)
300         CONTINUE
            S1(IP+Q,IP)=IPOS*ISUM
               S1(IP,IP+Q)=S1(IP+Q,IP)
            IPOS=-IPOS
400      CONTINUE

         QUP=2*NA+1-IP
         DO 450 Q=NZ,QUP
            S1(IP+Q,IP)=0
            S1(IP,IP+Q)=0
450      CONTINUE
500   CONTINUE

      ILOW=2*NA+2-NZ
      IUP=2*NA+1
      DO 700 IP=ILOW,IUP
         QUP=2*NA+1-IP
         DO 600 Q=0,QUP
            S1(IP+Q,IP)=0
            S1(IP,IP+Q)=0
600      CONTINUE
700   CONTINUE

      CALL FACTORIAL(NZ,PZ)

      MFACT=M-2*NA-NZ
      IUP=2*NA+1
      DO 1500 IP=1,IUP
         DO 1300 Q=1,NZ
            INDEX=IP+Q
            IF (INDEX.GT.IUP) GOTO 1290
            S2(IP+Q,IP)=MFACT*PZ(Q)
            S2(IP,IP+Q)=S2(IP+Q,IP)
1290           CONTINUE
1300           CONTINUE
         S2(IP,IP)=MFACT*PZ(NZ+1)
         QUP=2*UA+1-IP
         QLOW=NZ+1
         DO 1400 Q=QLOW,QUP
            S2(IP+Q,IP)=0
            S2(IP,IP+Q)=0
1400           CONTINUE
1500        CONTINUE
```

```
      IUP=NA+1
      JUP=2*NA+1
      :DO 1700 I=1,IUP
        DO 1600 J=1,JUP
          K22(I,J)=S2(I,J)+2*S1(I,J)
1600      CONTINUE
1700    CONTINUE

      DO 2500 I=1,NA
        DO 2400 J=1,I
          Q22(I,J)=2*(K22(I,J)+K22(I,2*NA+2-J))
2400      CONTINUE
2500    CONTINUE

      DO 2700 J=1,NA
        Q22(NA+1,J)=K22(NA+1,J)+K22(NA+1,2*NA+2-J)
2700    CONTINUE

      Q22(NA+1,NA+1)=K22(NA+1,NA+1)

      RETURN
      END




      SUBROUTINE TMATRIX(T,NA,NZ)
      INTEGER T(40,1),KF(40)

      CALL FACTZ(NZ,KF)
      DO 500 I=1,NA
        DO 400 J=1,I
          ISUM=O
          ISIGN=1
          IJ=I+J
          IF ((IJ/2)*2.NE.IJ) ISIGN=-1
          DO 300 K=1,NA
           IMK=I-K
           IF (IMK.GT.NZ)IFACT1=0
           IF (IMK.LT.O).IFACT1=0
           IF (IMK.EQ.O) IFACT1=1
           IF (IMK.GT.O .AND.IMK.LE.NZ)IFACT1=KF(IMK)
           JMK=J-K
           IF (JMK.GT.NZ)IFACT2=0
           IF (JMK.LT.O) IFACT2=0
           IF (JMK.EQ.O) IFACT2=1
           IF (JMK.GT.O .AND. JM.X.LE.NZ)IFACT2=KF(JMK)
           ISUM=[SlJM+IFACT1 *IFACT2
300       CONTINUE
          T(I,J)=ISIGN*ISUM
400     CONTINUE
500 CONTINUE

      RETURN
      END
```

```
      SUBROUTINE QMAT21 (Q21,NA,NZ)
      INTEGER Q21(41,1),U(40,6),R(40,15),K12(2420,81),PSI(80)

      CALL FACTORIAL(NZ,PSI)

      CALL UVECTORS(U,NZ,NA,PSI)

      CALL RMATRICES(U,R,NZ,NA)

      CALL KMAT12(K12,R,NZ,NA)

      IUP=NA*(3*NA+1)/2

      DO 200 I=1,IUP
         DO 100 J=1,NA
            Q21(J,I)=2*(K12(I,J)+K12(I,2*NA+2-J))
100      CONTINUE
         Q21(NA+1,I)=2*K12(I,NA+1)
200   CONTINUE

      RETURN
      END




      SUBROUTINE FACTORIAL(N,KF)
      INTEGER N,KF(1)

C     CALC OF FACTORIALS  (2N OVER N), (2N OVER N-1),•••(2N OVER 0)
C     RESULT STORED AS KF(J) = (-1)**J *(2N OVER N-J)    FOR   J=1,2•••N
C     KF(O) = (2N OVER N) IS STORED IN KF(N+1)

      NR=(N/2)*2-N
      ISIGN=1
      IF(NR.NE.O) ISIGN=-1

      KF(N)=ISIGN
      N1=N-1
      DO 100 K=1,N1
         INDEX=N-K+1
         KF(INDEX-1)=-KF(INDEX)*(2*N-K+1)/K
100   CONTINUE

      KF(N+1)=KF(1)*(N+1)/N
      IF (KF(N+1).LT.O) KF(N+1)=-KF(N+1)

      RETURN
      END
```

```
      SUBROUTINE FACTZ(N,KF)
      INTEGER KF(1)

C     CALC OF FACTORIALS (N OVER I)I=1,••• N
C     KF(I)= (N OVER I) I=1,••• N

      KF(1)=N
      IF (N.EQ.1)GOTO 200
      DO 100 K=2,N
         KF(K)=KF(K-1)*(N-K+1)/K
100   CONTINUE
200   CONTINUE

      RETURN
      END
```

```
      SUBROUTINE UVECTORS (U,NZ,NA,PSI)
      INTEGER U(40,1),PSI(1)

C     CALC OF THE VECTORS U(J) J=1,••• Z
C     U(J) = (O,••• O,PSI(NZ),••• PSI(J) )**T
C     THE VECTORS ARE STORED COLUMNWISE IN THE MATRIX U
C     AS U= (U(1),U(2),••• U(NZ) )

      DO 1000 J=1,NZ

         NUP=NA+J-NZ-1
         DO 100 I=1,NUP
100         U(I,J)=O

         NLOW=NUP+1
         INDEX=NZ
         DO 200 I=NLOW,NA
            U(I,J)=PSI(INDEX)
            INDEX=INDEX-1
200         CONTINUE

1000        CONTINUE

      RETURN
      END
```

```
      SUBROUTINE RMATRICES(U,R,NZ,NA)
      INTEGER U(40,1),R(40,1)

C     CALC OF R-MATRIX
C     R(P)= (U(P),U(P-1),••• U(1) )   P=1,2,••• NZ
C     THE MATRICES ARE STORED IN THE LARGE R-MATRIX
C     R= (R(1),R(2),•••  R(NZ))

      JCOLR=0
      DO 500 JP=1,NZ
         DO 400 J=1 ,JP
            JCOLR=JCOLR+1
            JCOLU=JP-J+1
            DO 300 I=1,NA
               R (I,JCOLR)=U (I,JCOLU)
300         CONTINUE
400      CONTINUE
'100  CONTINUE

      RETURN
      END




      SUBROUTINE KMAT12(K12,R,NZ,NA)
      INTEGER K12(2420,1),R(40,1),RCOL

C     CALC OF THE MATRIX K12

      IUP=NA*(NA+1 )+NA*(NA-1 )/2
      JUP=2*NA+1
      DO 100 I=1,IUP
         DO 100 J=1,JUP
            K12(I,J)=0
100   CONTINUE

      DO 500 IP=1 ,NZ
         KROWLOW= (IP-1 )*NA
         RCOL=IP(IP-1)/2
         DO 400 J=1,IP
           RCOL=RCOL+1
           KROW=KROWLOW
           DO 300 I=1,NA
             KROW=KROW+1
             K12(KROW,J)=R(I,RCOL)
300        CONTINUE
400      CONTINUE
500   CONTINUE
```

```
      IPLOW'=NZ+l
      IPUP=NA+1
      DO 1500 IP=IPLOW,IPUP
         KROWLOW=(IP-1)*NA
         RCOL=(NZ-1)*NZ/2
         JLOW=IP-NZ+1
         JUP=JLOW+NZ-1
         DO 1400 J=JLOW,JUP
            RCOL=RCOL+1
            .KROW=KROWLOW
            DO 1300 I=1,NA
               KROW=KROW+1
               K12(KROW,J)=R(r;acoL)
1300           CONTINUE
1400        CONTINUE
1500     CONTINUE

      IPLOW=NA+2
      IPUP=2*NA
      DO 2500 IP=IPLO,IPUP
         NY=IP-(NA+1)
         KROWLOW=(NA+1)*NA+(NY-1)*NA-NY*(NY-1)/2
         RCOL=(NZ-1)*NZ/2
         JLOW=IP-NZ+1
         JUP=JLOW+NZ-1
         DO 2400 J=JLOW,JUP
           RCOL=RCOL+1
           KROW=KROWLOW
           ILOW=IP-NA
           DO 2300 I=ILOW,NA
              KROW=KROW+1
              K12(KROW,J)=R(I,RCOL)
2300          CONTINUE
2400       CONTINUE
2500     CONTINUE

      RETURN
      END
```

5.3 The subroutine CONSTRAINT

```
      SUBROUTINE CONSTRAINT(V,HL,D,A,NOCONSTR,LOWV,UPV,INDV,
     *  LOWCOL,UPCOL,COLIN,GIVENR)
      REAL*8 V(2461,1),HL(1)
      INTEGER D,A,LOWV(1),UPV(1),INDV(1),LOWCOL(1),UPCOL(1),COLIN(1)
      LOGICAL GIVENR
      INTEGER LOW,LOWHL,UP,I,J,IP
      REAL*8 FI(81,6)

      LOWHL=0
      UP=0
      LOW=1
      DO 300 IP=1,A
         NROW=A+IP
         UP=UP+NROW
         CALL ORTBASIS(NROW,D,FI)

         DO 200 I=1,D
            INDEX=1
            DO 190 J=LOW,UP
             V(J,I)=FI(INDEX,I)
               INDEX=INDEX+1
190         CONTINUE
            LI=LOWHL+I
            HL(LI)=FI(IP,I)
            LOWV(LI)=LOW
           UPV(LI)=UP
           INDV(LI)=I
200      CONTINUE

         DO 250 J=LOW,UP
            CALL NEWINDEX(J,IP,A,JNEW)
            COLIN(J)=JNEW
            LOWCOL(J)=LOWHL+1
            UPCOL(J)=LOWHL+D
250      CONTINUE

         LOWHL=LOWHL+D
         LOW=LOW+NROW
300   CONTINUE
```

```
      LOW=UP+1
      UP=LOW+A-1
      NROW=2*A+1

      CALL ORTBASIS(NROW,D,FI)

      IVCOL=1
      DO 500 I=1,D
         INDEX=1
         IF ((I-(I/2)*2).EQ.O) GOTO 495
         DO 490 J=LOW,UP
            V(J,IVCOL)=FI(INDEX,I)+FI(2*A+2-INDEX,I)
            INDEX=INDEX+1
490      CONTINUE
         LI=LOWHL+IVCOL
         HL(LI)=FI(A+1,I)
         V(UP+1,IVCOL)=FI(A+1,I)
         LOWV(LI),.LOW
         UPV (LI)=UP+1
         INDV(LI)=IVCOL
         IVCOL=IVCOL+1
495      CONTINUE
500   CONTINUE

      NOCONSTR=LOWHL+IVCOL-1

      UP=UP+1
      DO 600 J=LOW,UP
         COLIN (J)=J
         LOWCOL(J)=LOWHL+1
         UPCOL(J)=NOCONSTR
600   CONTINUE

      IF (GIVENR) NOCONSTR=A*D

      RETURN
      END




      SUBROUTINE ORTBASIS(M,D,FI)
      REAL*S FI(81,1),GAMMA,BETA,CAPPA,SUM,SUMX,TERM,SUMNX
      INTEGER D,D1

C     FIND AN ORTHOGONAL BASIS FOR THE SPACE OF POLYNOMIALS OF


C     DEGREE LESS THAN D. THE ORTOGONALITY IS WITH RESPECT TO
C     THE INNERPRODUCT
C           <F,G>= f(1)*g(1)+•••  f(M)*g(M)
C     THE RESULT IS A SET OF ORTHOGONAL VECTORS STORED COLUMNWISE
C     IN THE UPPER LEFT CORNER OF THE MATRIX  FI.
```

```
      SUM=0
      SUMX=0
      SUMNX=0
      GAMMA=(M+1)/2D0
      CAPPA=SQRT(M/1D0)

      DO 100 I=1,M
         FI(I,1)=1D0/CAPPA
         FI(I,2)=I-GAMMA
         TERM=FI(I,2)*FI(I,2)
         SUM=SUM+TERM
         SUMX=SUMX+I*TERM
         SUMNX=SUMNX+I*FI(I,1)*FI(I,2)
100   CONTINUE

      D1=D-1
      DO 500 N=2,D1
         CAPPA=SQRT(SUM)
         BETA=SUMX/SUM
         GAMMA=SUMNX/CAPPA
         SUM=0
         SUMX=0
         SUMNX=0
         DO 400 I=1,M
            FI(I,N)=FI(I,N)/CAPPA
            FI(I,N+1)=(I-BETA)*FI(I,N)-GAMMA*FI(I,N-1)
            TERM=FI(I,N+1)**2
            SUM=SUM+TERM
            SUMX=SUMX+TERM*I
            SUMNX=SUMNX+I*FI(I,N+1)*FI(I,N)
400      CONTINUE
500   CONTINUE

      RETURN
      END




      SUBROUTINE NEWINDEX(ININD,T,A,OUTIND)
      INTEGER ININD,T,A,OUTIND

      J=LIND-(T-1)*A-T*(T-1)/2
      IF(J.LT.(A+2))GOTO 100

      OUTIND=(J-1)*A+T-(J-A)*(J-A-1)/2
      RETURN

100   CONTINUE
      OUTIND=(J-1)*A+T
      RETURN
      END
```

5.4 Input and output subroutines

```
      SUBROUTINE GIVEDATA (A,D,Z,M,R,GIVENR)
      REAL*8 R(l)
      INTEGER A,D,Z,M,Al,G
      LOGICAL GIVENR
      CHARACTER*1 ANS
      CHARACTER*15 INFILE

      WRITE(5,11)
11    FORMAT('The no. of points in the main moving average is 2*a+1 .'
     * ,/,' (1<=a<=40),/,' Give tail length a: )

      READ(5,15) A


15    FORMAT(I)

      WRITE(5,21)
21    FORMAT('The graduation method will be exact for polynomials of '
     * ,/,' degree G (<=5 and <=a).,/,' Give G: )
      READ(5,15) G
      D=G+1

      WRITE(5,31)
31    FORMAT('The object function contains a difference af order z.',
     * /,' (1<=z<=5 and z<a ),/,' Give z: )
      READ(5,15) Z

      WRITE(5,41)
41    FORMAT('The no. of observations is m (>2*a+z).,/,' Give m: )
      READ(5,15) m


      WRITE(5,101)
101   FORMAT('Coefficients af the main moving average known?(YES/NO))
      READ(5,102) ANS
102   FORMAT(A)
      IF(ANS.EQ.Y'.OR.ANS.EQ.y'.OR. ANS.EQ.J'.OR. ANS.EQ.j)
     * GOTO 200
      GOTO 1000
```

```
200 CONTINUE

    WRITE(5,208)
208 FORMAT('Give the name of the file of the r-coefficients : )

C   In the file the coefficients must be stored as
C      r<1>
C      r<2>
C
C
C
C   r<a+1>
C   i.e. sequentially with one value on each row.
C   The numbers must contain a decimal point, i.e. even if the
C   value is 5500 it must be given as 5500.0.
C   If r<a+1> is greater than 1 the program assumes that the
C   coefficients in the file are scaled by the factor 10**I
    where I is a positive integer. In that case the file is
    terminated with one row containing the integer I.

    READ (5,209)INFILE
209 FORMAT(A)

    OPEN(UNlT=9,FILE=INFILE,STATUS= OLD )

    GIVENR=.TRUE.
    A1 =A+1
    READ(9,302) (R(I),I=1,A1 )
302 FORMAT(F)

    IF(R(A1).LE.1DO) GOTO 400

    READ (9,307)ISCALE
307      FORMAT(I)

    MSCALE=f
    DO 320 I=1,ISCALE
320 MSCALE=MSCALE*1O

    DO 350 I=1 ,A1
350 R(I)=R(I)/MSCALE



400 CONTINUE

1 000     CONTINUE

    RETURN
    END
```

```
      SUBROUTINE OUTCOEF(X,QSUM,A,D,Z ,M,LOWV,UPV,INDROW,GIVENR)
      REAL*8 X(1),QSUM
      INTEGER A,D,Z,M,LOWV (1 ),UPV (1 ),INDROW (1 )
      INTEGER A1 ,A2,OUTMAT (81 ,41 )
      LOGICAL GIVENR
      CHARACTER*1 1 RFILE
      CHARACTER *1 GP

C     CREATE A FILENAME AND FILE FOR OUTPUT OF RESULTS
C     !THIS IS NOT STANDARD FORTRAN !

      LED=Z*100+2*A+1
      ND=D-1
      IF (ND .EQ .0) GP= 0 '
      IF (ND.NE.O) WRITE(GP,5) ND
5     FORMAT (I1 )
      IF (.NOT.GIVENR) WRITE(RFILE,10)GP,LED,M
      IF (GIVENR)      WRITE(RFILE,20)GP,LED
10 FORMAT(FRI ,A1,I3, .I3)
20 FORMAT(FST ,A1,I3, .KFF )
      OPEN (UNIT=8,FILE=RFILE,STATUS= NEW )

C     PREPARE DATA FOR PRINTING

      A1 =A+1
      A2=2*A+1
      DO 200 I=1 ,A2
         DO 190 J=1,A1
            OUTMAT (I,J)=0
190      CONTINUE
200 CONTINUE


      DO 400 J=1 ,A1
         IND=(J-1)*D+1
         LOW=LOWV(IND)
         UP=UPV(IND)
         DO 300 I=LOW,UP
            OUTMAT (I-LOW+1 ,J )=NINT (X (INDROW (I ) )*1 00000 )
300      CONTINUE
400 CONTINUE

      DO 500 I=1,A
         OUTMAT(2*A+2-I,A1 )=OUTMAT(I,A1 )
500 CONTINUE

      DO 700 I=1 ,A2
         WRITE(8,709) (OUTMAT(I,J),J=1,A1 )
700 CONTINUE
709 FORMAT (11 I8)

      WRITE (S,709)
      IF ( .NOT .GIVENR) WRITE (S,719 ) QSUM
719 FORMAT ( 'TRACE=',E15 .6)

      WRITE(S,809)RFILE
809 FORMAT( ' For results, see file ',A11 )

      RETURN
      END
```

APPENDIX 1. Contruction of Q

Here is a safe way of stepwise construction of the matrix Q. This algorithm was given by Hoem (1983).

Let

$$T_{ij} \equiv (-1)^{i+j} \sum_{k=1}^{a} \binom{z}{i-k}\binom{z}{j-k},$$

for $i = 1, 2, \ldots, a$, and $j = 1, 2, \ldots, a$, and let

$$F_p = T, \quad \text{for } p = 1, 2, \ldots, a+1,$$

$$F_p = \{T_{ij}: i,j = p-a, p-a+1, \ldots, a\} \quad \text{for } p = a+2, \ldots, 2a.$$

Then define

$$K_{11} = \text{diag } \{F_1, F_2, \ldots, F_{2a}\}.$$

Note that K_{11} has a dimension $\frac{1}{2}a(3a+1)\times\frac{1}{2}a(3a+1)$. Let

$$\psi_j = (-1)^j \binom{2z}{z-j}$$

for integer j, and note that $\psi_j = 0$ for $j > z$. Define

$$\underline{\underline{u}}_j = (\psi_{j+a-1}, \psi_{j+a-2}, \ldots, \psi_j)^T \quad \text{for } j = 1, 2, \ldots, z.$$

Then $\underline{\underline{u}}_j$ is a column vector with $\underline{a}$ components. Also let

$$R_p = \begin{cases} (\underline{\underline{u}}_p, \underline{\underline{u}}_{p-1}, \ldots, \underline{\underline{u}}_1), & \text{for } p = 1, 2, \ldots, z-1, \\ (\underline{\underline{u}}_z, \underline{\underline{u}}_{z-1}, \ldots, \underline{\underline{u}}_1), & \text{for } p = z, z+1, \ldots, 2a+1. \end{cases}$$

Note that

$$\underline{\underline{u}}_j = (0, \ldots, \underline{0}, \psi_z, \psi_{z-1}, \ldots, \psi_j)^T,$$

with a+j-z-1 leading zeros, so a lot of the elements of each R_p are 0.

Now let $C_p = R_p$ for $p = 1, 2, \ldots, a+1$, while for $p > a+1$ we define C_p as R_p with the p-a-1 first rows omitted:

$$C_p = \begin{cases} R_p, & \text{for } p = 1, 2, \ldots, a+1, \\ \left\{ (R_p)_{ij};\ \begin{matrix} i = p-a,\ p-a+1,\ \ldots,\ a; \\ j = 1, 2, \ldots, z \end{matrix} \right\}, & \text{for } p = a+2, \ldots, 2a. \end{cases}$$

Now define

$$\bar{C}_p = \begin{cases} \{C_p,\ 0(a,\ 2a+1-p)\}, & \text{for } p = 1, 2, \ldots, z, \\ \{0(a,p-z),\ C_p, 0(a, 2a+1-p)\}, & \text{for } p = z+1, \ldots, a+1, \\ \{0(2a+1-p,\ p-z), C_p,\ 0(2a+1-p,\ 2a+1-p)\}, & \text{for } p = a+2, \ldots, 2a. \end{cases}$$

Here $0(m,n)$ is an $m \times n$ matrix all of whose elements are zero. Then $\bar{C}_p$ has 2a+1 columns.

Let

$$K_{12} = \begin{bmatrix} \bar{C}_1 \\ \bar{C}_2 \\ \cdot \\ \cdot \\ \cdot \\ \bar{C}_{2a} \end{bmatrix}, \text{ and } K_{21} = K_{12}^{\ T}.$$

Then K_{12} is a $\frac{1}{2}a(3a+1) \times (2a+1)$ matrix. Let S_1 be a symmetric $(2a+1)\times(2a+1)$ matrix with elements

$$(S_1)_{p,p+q} = \begin{cases} (-1)^q \sum\limits_{j=1}^{z-q} j\binom{z}{j}\binom{z}{j+q}, & \text{for } q = 0, 1, \ldots, z-1, \\ 0, & \text{for } q = z, z+1, \ldots, 2a+1-p, \end{cases}$$

when $p = 1, 2, \cdots, 2a+1-z$. For $p = 2a+2-z, \cdots, 2a+1$, and $q = 0, 1, \cdots, 2a+1-p$, $(S_1)_{p,p+q}$ is again defined by the above summation formula. Also let S_2 be a symmetric $(2a+1)\times(2a+1)$ matrix defined by

$$(S_2)_{p,p+q} = (m-2a-z)(-1)^q \binom{z}{q},$$

for $q = 0, 1, \cdots, 2a+1-p$, and $p = 1, 2, \cdots, 2a+1$. Note that $(S_2)_{p,p+q} = 0$ for $q > z$. As before, the parameter m represents the number of observation points on the curve which is to be smoothed.

Finally, let $K_{22} = S_2 + 2S_1$ and

$$K = \begin{vmatrix} K_{11}, & K_{12} \\ K_{21}, & K_{22} \end{vmatrix}$$

The matrix Q can now be obtained from K in the following way:

Partition Q as

$$Q = \begin{vmatrix} Q_{11}, & Q_{12} \\ Q_{21}, & Q_{22} \end{vmatrix}$$

with $Q_{21} = Q_{12}^T$, Q_{11} a symmetric $a(3a+1) \times a(3a+1)$ matrix, and Q_{22} a symmetric $(a+1)\times(a+1)$ matrix. Thus Q_{12} has dimension $a(3a+1)\times(a+1)$.

Furthermore,

$$Q_{11} = 2K_{11},$$

$$(Q_{12})_{ij} = \begin{cases} 2\{(K_{12})_{ij} + (K_{12})_{i,2a+2-j}\}, & \text{for } j = 1, 2, \ldots, a, \\ 2(K_{12})_{i,a+1}, & \text{for } j = a+1, \end{cases}$$

for $i = 1, 2, \cdots, a(3a+1)$.

Also,

$$(Q_{22})_{ij} = \begin{cases} 2\{(K_{22})_{ij} + (K_{22})_{i,2a+2-j}\}, & \text{for} \begin{cases} i = 1, 2, \ldots, a, \\ j = 1, 2, \ldots, a, \end{cases} \\ (K_{22})_{a+1,j} + (K_{22})_{a+1,2a+2-j}, & \text{for} \begin{cases} i = a+1, \\ j = 1, 2, \ldots, a, \end{cases} \\ (K_{22})_{a+1,a+1}, & \text{for} \begin{cases} i = a+1, \\ j = a+1, \end{cases} \\ (K_{22})_{a+1,i} + (K_{22})_{a+1,2a+2-i}, & \text{for} \begin{cases} i = 1, 2, \ldots, a, \\ j = a+1. \end{cases} \end{cases}$$

APPENDIX 2. NAG library routines

The following subroutines from the NAG library, Mark 9, have been used:

F01MCF,

F04MCF,

F04ASF.

Descriptions of the routines can be found in the NAG library manuals.

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