

CALCULATION OF INTERPOLATING NATURAL SPLINE FUNCTIONS
USING DE BOOR'S PACKAGE FOR CALCULATING WITH B-SPLINES

by

John G. Herriot

STAN-CS-76-569

OCTOBER 1976

COMPUTER SCIENCE DEPARTMENT
School of Humanities and Sciences
STANFORD UNIVERSITY



Calculation of Interpolating Natural Spline Functions
Using de Boor's Package for Calculating with B-Splines

by

John G. Herriot

Computer Science Department
Stanford University
Stanford, California 94305

Abstract.

A FORTRAN subroutine is described for finding interpolating natural splines of odd degree for an arbitrary set of data points. The subroutine makes use of several of the subroutines in de Boor's package for calculating with B-splines. An ALGOL W translation of the interpolating natural spline subroutine and of the required subroutines of the de Boor package are also given. Timing tests and accuracy tests for the routines are described.

The work of this author was supported in part by the National Science Foundation under grant number MCS71-01996-A06.

Table of Contents

1.	Introduction	1
2.	B-Splines	3
3.	Representation of the Interpolating Spline	8
4.	The FORTRAN Subroutine	14
5.	The ALGOL W Procedure	20
6.	Tests	22
	References	28
	Appendix I	29
	Appendix II	37

We now explain how a piecewise polynomial function can be expressed as a linear combination of B-splines. Let $\xi = (\xi_i)_{i=1}^{\ell+1}$ be a strictly increasing real sequence and let k be a positive integer. If P_1, \dots, P_ℓ is any sequence of ℓ polynomials, each of order k (or, degree $< k$) then we define a corresponding piecewise polynomial f of order k by the prescription

$$f(t) = P_i(t) \quad \text{if } \xi_i < t < \xi_{i+1} ; \quad i = 1, 2, \dots, \ell .$$

We arbitrarily make f continuous from the right at the interior breakpoints, i.e.,

$$f(\xi_i) = f(\xi_i^+) \quad \text{for } i = 2, \dots, \ell .$$

We denote the collection of all such piecewise polynomial functions of order k with breakpoint sequence $\xi = (\xi_i)_{i=1}^{\ell+1}$ by

$$\mathbb{P}_{k, \xi} .$$

Note that $\mathbb{P}_{k, \xi}$ is a linear space of dimension $k\ell$ since it is isomorphic to the direct product of ℓ copies of \mathbb{P}_k , the linear space of all polynomials of order k (degree $< k$). A convenient way to represent a piecewise polynomial function $f \in \mathbb{P}_{k, \xi}$ is by

$$f(t) = \sum_{r=1}^k c_{r,i} (t - \xi_i)^{r-1} , \quad \xi_i \leq t < \xi_{i+1} , \quad i = 1, 2, \dots, \ell \quad (2.7)$$

where $c_{r,i} = D^{r-1} f(\xi_i^+) / (r-1)!$, $r = 1, \dots, k$; $i = 1, \dots, \ell$. Then the j -th derivative of f at a point t is given by

$$D^j f(t) = \sum_{r=j+1}^k c_{r,i} (t - \xi_i)^{r-1-j} (r-1)! / (r-1-j)! . \quad (2.8)$$

We often wish to impose upon f the conditions that it have a certain number of continuous derivatives. We may write such conditions in the form

$$\text{jump}_{\xi_i} D^{j-1} f = 0, \quad \text{for } j = 1, \dots, v_i, \quad i = 2, \dots, l \quad (2.9)$$

for some vector $v = (v_i)_2^\ell$ with nonnegative integer entries. The subset of all $f \in \mathbb{P}_{k, \xi}$ satisfying (2.9) for a given v is a linear subspace of $\mathbb{P}_{k, \xi}$ which we denote by $\mathbb{P}_{k, \xi, v}$.

In order to obtain the B-spline representation of a piecewise polynomial function $f \in \mathbb{P}_{k, \xi, v}$ we need the following theorem which was proved by Curry and Schoenberg [5] and by de Boor [4].

Theorem. For a given strictly increasing $\xi = (\xi_i)_1^{\ell+1}$, and given nonnegative integer sequence $v = (v_i)_2^\ell$, with $v_i < k$, all i , set

$$n = k + \sum_{i=2}^{\ell} (k - v_i) = k\ell - \sum_{i=2}^{\ell} v_i = \dim \mathbb{P}_{k, \xi, v} \quad (2.10)$$

and let $t = (t_i)_1^{n+k}$ be any non-decreasing sequence so that

$$(i) \quad t_1 \leq t_2 \leq \dots \leq t_k \leq \xi_1, \quad \xi_{\ell+1} \leq t_{n+1} \leq t_{n+k}$$

(ii) for $i = 2, \dots, \ell$, the number ξ_i occurs exactly $k - v_i$ times in t .

Then the sequence $N_{1,k}, \dots, N_{n,k}$ of B-splines of order k (or degree $k-1$) corresponding to the knot sequence t is a basis for $\mathbb{P}_{k, \xi, v}$ considered as functions on $[t_k, t_{n+1}]$.

From this theorem we see that the B-spline representation for the piecewise polynomial function $f \in \mathbb{P}_{k, \xi, v}$ is

$$f(t) = \sum_{r=i-k+1}^i a_r N_{r,k}(t), \quad \begin{cases} t_i \leq t < t_{i+1} & \text{and } k < i < n \\ \text{or } t_i \leq t \leq t_{i+1} & \text{and } i = n \end{cases} \quad (2.11)$$

where $a = (a_i)_1^n$ are the coefficients of f with respect to the B-spline

basis $(N_{i,k})_1^n$ for $\mathbb{P}_{k,y}$ on the knot sequence t . Then the j -th derivative of f at a point t is given by

$$D_j f(t) = \sum_{r=i-k+j+1}^i a_{r,j+1} N_{r,k-j}(t) \quad (2.12)$$

where

$$a_{r,j+1} = \begin{cases} a_r & , \quad j = 0 \\ (k-j) \frac{a_{rj} - a_{r-1,j}}{t_{r+k-j} - t_r} & , \quad j > 0 \end{cases} \quad (2.13)$$

provided that either $t_i < t < t_{i+1}$ and $k \leq i < n$
or $t_i \leq t \leq t_{i+1}$ and $i = n$.

3. Representation of the Interpolating Spline.

Given a set of data points (x_i, y_i) , $i = N_1, N_1+1, \dots, N_2$ with $x_{N_1} < x_{N_2} < \dots < x_{N_2}$, we seek the interpolating natural spline function $S(x)$ of degree $2m-1$ with knots x_{N_1}, \dots, x_{N_2} . For convenience in the FORTRAN implementation of the algorithm we shall assume throughout that $N_1 = 1$. Then N_2 is the number of data points. For our interpolating natural spline $S(x)$ we wish to make use of the B-spline representation given in equation (2.11) and the theorem on which it is based. We choose $k = 2m$, $l = N_2 - 1$. Since $D^{j-1}S(x)$, $j = 1, 2, \dots, 2m-1$, are continuous at all interior knots, we have $v_i = 2m-1$, all i , and we easily find that $n = N_2 + 2m - 2$. We choose

$$\begin{aligned} t_i &= x_1, & i &= 1, 2, \dots, 2m \\ t_{2m+i-1} &= x_1, & i &= 2, 3, \dots, N_2-1 \\ t_{N_2+2m+i-2} &= x_{N_2}, & i &= 1, 2, \dots, 2m \end{aligned} \quad (3.1)$$

The knot distribution is shown in Figure 1.

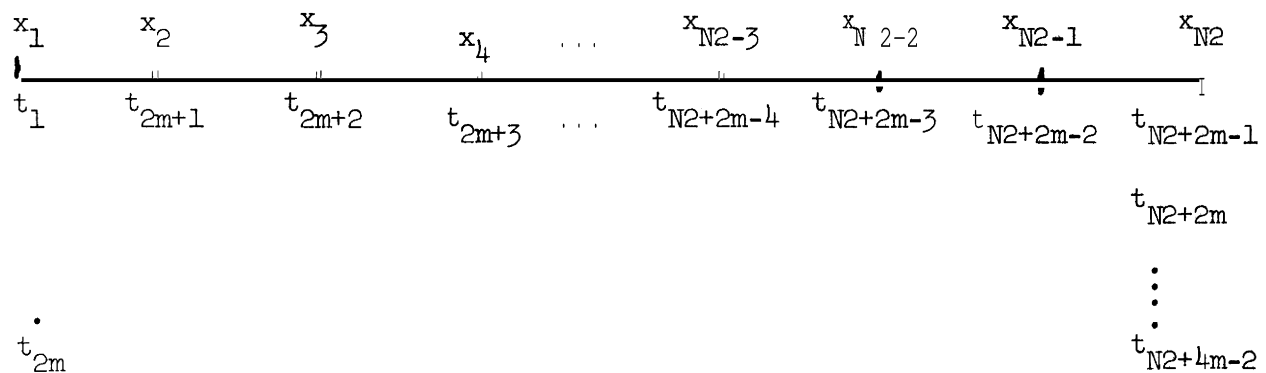


Figure1

From equation (2.11) we have the B-spline representation

$$S(t) = \sum_{r=i-2m+1}^i a_r N_{r,2m}(t) \begin{cases} t_i \leq t < t_{i+1} & \text{and } 2m < i < N2+2m-2 \\ \text{or} \\ t_i \leq t \leq t_{i+1} & \text{and } i = N2+2m-2 \end{cases} . \quad (3.2)$$

Now $S(x)$ must satisfy the interpolating conditions

$$S(x_i) = y_i , \quad i = 1, 2, \dots, N2 \quad (3.3)$$

and the natural spline end conditions

$$D^j S(x_1) = D^j S(x_{N2}) = 0 , \quad j = m, m+1, \dots, 2m-2 \text{ if } m > 1 . \quad (3.4)$$

Substituting equation (3.2) into equations (3.3) and (3.4) we obtain the following set of equations for the determination of the a_r :

$$D^j S(x_1) = \sum_{r=1}^{2m} a_r D^j N_{r,2m}(x_1) = 0 , \quad j = m, m+1, \dots, 2m-2 \quad (3.5)$$

$$S(x_i) = \sum_{r=i}^{2m+i-1} a_r N_{r,2m}(x_i) = y_i , \quad i = 1, 2, \dots, N2 \quad (3.6)$$

$$D^j S(x_{N2}) = \sum_{r=N2-1}^{N2+2m-2} a_r D^j N_{r,2m}(x_{N2}) = 0 , \quad j = m, m+1, \dots, 2m-2 . \quad (3.7)$$

We now show that these equations lead to a $(2m-1)$ -banded system of linear equations for the determination of the a_r . In Section 2 it was pointed out that $N_{r,2m}(t)$ is positive for $t_r < t < t_{r+2m}$ and zero otherwise. From equation (2.5) we conclude that at a knot t_j of multiplicity d_j , $D^s N_{r,2m}(t)$ is continuous for $s = 0, 1, \dots, 2m-1-d_j$. In-particular, if $d_j = 2m-1$, then $N_{r,2m}(t)$ is continuous at t_j but none of its derivatives is continuous at t_j . If $d_j = 2m$, then even $N_{r,2m}(t)$ is discontinuous at t_j . For the coefficients in equations (3.6) we therefore conclude that

$$N_{1,2m}(x_1) \neq 0, \quad N_{r,2m}(x_1) = 0, \quad r = 2, 3, \dots, 2m$$

$$\left. \begin{array}{l} N_{2m+i-1,2m}(x_i) = 0 \\ N_{r,2m}(x_i) \neq 0, \quad r = 1, \dots, 2m+i-2 \end{array} \right\} \quad i = 2, 3, \dots, N_2-1$$

$$N_{N_2+2m-2,2m}(x_{N_2}) \neq 0, \quad N_{r,2m}(x_{N_2}) = 0, \quad r = N_2, \dots, N_2+2m-3.$$

For the coefficients in equation (3.5) we find that

$$\left. \begin{array}{l} D^j_{r,2m}(x_1) \neq 0, \quad r = 1, 2, \dots, j+1 \\ = 0, \quad r = j+2, \dots, 2m \end{array} \right\} \quad j = m, m+1, \dots, 2m-2$$

and for the coefficients in (3.7)

$$\left. \begin{array}{l} D^j_{r,2m}(x_{N_2}) = 0, \quad r = N_2-1, \dots, N_2+2m-3-j \\ \neq 0, \quad r = N_2+2m-2-j, \dots, N_2+2m-2 \end{array} \right\} \quad j = m, \dots, 2m-2.$$

If we denote the non-zero coefficients of the system of equations given by (3.5), (3.6), (3.7) by x , then the coefficient matrix has the form:

[illegible]

We have boxed the coefficients of a_1 and $a_{N2+2m-2}$ to emphasize the fact that these two coefficients can be calculated at once and eliminated from the remaining equations yielding a banded matrix with $m-1$ subdiagonals and $m-1$ superdiagonals. We use the first and last equations of (3.6) to obtain

$$a_1 = y_1 / N_{1,2m}(x_1)$$

$$a_{N2+2m-2} = y_{N2} / N_{N2+2m-2,2m}(x_{N2}) .$$

Then from (3.5) and (3.7) we have

$$\sum_{r=2}^{j+1} A_r D^j N_{r,2m}(x_1) = -a_1 D^j N_{1,2m}(x_1) \quad (3.8)$$

$$j = m, m+1, \dots, 2m-2$$

and

$$\sum_{r=N2+2m-2-j}^{N2+2m-3} A_r D^j N_{r,2m}(x_{N2}) = -a_{N2+2m-2} D^j N_{N2+2m-2,2m}(x_{N2}) \quad (3.9)$$

$$j = 2m-2, \dots, m .$$

The remaining equations are given by (3.6) with the first and last equations omitted. Now we have a banded system; the unknowns are

$a_2, a_3, \dots, a_{N2+2m-3}$ which we rename $z_1, z_2, \dots, z_{N2+2m-4}$. We note that the diagonal elements of the system matrix are in order

$$D^m N_{2,2m}(x_1), D^{m+1} N_{3,2m}(x_1), \dots, D^{2m-2} N_{m,2m}(x_1),$$

$$N_{m+1,2m}(x_2), N_{m+2,2m}(x_3), \dots, N_{N2+m-3,2m}(x_{N2-1}),$$

$$D^{2m-2} N_{N2+m-1,2m}(x_{N2}), D^{2m-3} N_{N2+m,2m}(x_{N2}), \dots, D^m N_{N2+2m-3,2m}(x_{N2}).$$

The subdiagonal and superdiagonal elements are also values and derivatives of B-splines evaluated at the knots.

All the elements of this matrix are calculated by using the subroutines of de Boor's B-spline package [4]. The elements of the matrix are stored in diagonal form for use of the band matrix solver subroutines `BANDET` and `BANDSL` which are essentially FORTRAN implementations of the corresponding ALGOL 60 procedures given by Martin and Wilkinson [10]. The diagonal elements are stored as $Q(i,m)$, the subdiagonal elements as $Q(i,j)$, $j = 1, 2, \dots, m-1$, the superdiagonal elements as $Q(i,j)$, $j = m+1, m+2, \dots, 2m-1$, where $i = 1, 2, \dots, N+2m-4$.

The solution of this system of equations yields the coefficients a_r of the B-spline representation (3.2) for the interpolating natural spline $S(t)$. The values of $S(t)$ and its derivatives can be evaluated at any point by means of subroutines in the de Boor package. In particular we can obtain the piecewise polynomial representation (2.7) (or (1.1)) of $S(x)$ by evaluating the function and the derivatives at the breakpoints.

4. The FORTRAN Subroutine.

Before describing the FORTRAN subroutine NATSPP for the interpolating natural spline we first describe briefly those subroutines of the de Boor package [4] which are used in the subroutine NATSPP.

We begin with a summary of the FORTRAN variables and their intended use and a terse summary of the subprograms and their intended use,

The B-spline representation consists of

$T(1), \dots, T(N+K)$, the **knot** sequence, assumed nondecreasing; if t appears j times in this sequence, then the $(K-j)$ -th derivative may jump at t .

$A(1), \dots, A(N)$, B-spline coefficients for the function represented on $(T(K), T(N+1))$.

N , the number of B-splines of order K for the given knot sequence.

K , order (= degree +1) of the **B-splines**; should be < 20 .

The piecewise-polynomial representation consists of

$XI(1), \dots, XI(LXI+1)$, the breakpoint sequence, assumed increasing.

$C(1,1), \dots, C(K, LXI)$, values of derivatives at breakpoints; precisely

$C(J,I)$ is $(J-1)$ -st derivative at $XI(I)+$,

$J=1, \dots, K$. Note that the coefficients in (2.7)

and (1.1) are these derivatives divided by $(J-1)!$.

K , order (= degree +1) of polynomial pieces; should be ≤ 20 .

Other variables are defined in the subroutine summary which follows:

subroutine BSPLDR(T,A,N,K,ADIF,NDERIV)

Constructs divided difference table for B-spline coefficients preparatory to derivative calculation and stores it in ADIF(1,1), ..., ADIF(N,NDERIV) . Expects NDERIV in the interval [2,K] . Used only in BSPLPP, prior to call of BSPLEV.

subroutine BSPLEV(T,ADIF,N,K,X,SVALUE,NDERIV)

Calculates value of spline and its derivatives at X from B-spline representation and returns them in SVALUE(1), ... SVALUE(NDERIV) . Can use A for ADIF if NDERIV = 1 . Otherwise must have ADIF filled beforehand by BSPLDR. Uses INTERV and BSPLVN. Used only in BSPLPP.

subroutine BSPLPP(T,A,N,K,SCRTCH,XI,C,LXI)

Converts B-spline representation to piecewise-polynomial representation. SCRTCH is temporary storage of size (N,K) . Uses BSPLDR and BSPLEV. Used in NATSPP, the subroutine for natural spline interpolation.

subroutine BSPLVN(T,JHIGH,INDEX,X,ILEFT,VNIKX)

Calculates value of all possibly 'nonzero' B-splines at X of order $J = \max\{JHIGH, (J+1)*(INDEX-1)\}$ on T . ILEFT is input, assumed so that $T(ILEFT) < T(ILEFT+1)$; get division by zero otherwise. If $T(ILEFT) \leq X \leq T(ILEFT+1)$ (as would be expected) then VNIKX(I) is filled with B-spline value $N(ILEFT-J+I, J)$ at X , $I = 1, \dots, J$. Get limit from right or left, if $X = T(ILEFT)$ or $T(ILEFT+1)$ respectively. Can save time by using INDEX = 2 in case this call's desired order J is greater than the previous call's order (saved in J) provided T , X , ILEFT and VNIKX are unchanged between the calls. Otherwise, use INDEX = 1 . Used in BSPLEV, BSPLVD and NATSPP.

subroutine BSPLVD(T,K,X,ILEFT,VNIKX,NDERIV)

Calculates value and derivatives of order $< \text{NDERIV}$ of all B-splines which do not vanish at X . ILEFT is input, assumed so that $T(\text{ILEFT}) < T(\text{ILEFT}+1)$; get division by zero otherwise. If $T(\text{ILEFT}) \leq X \leq T(\text{ILEFT}+1)$ (as would be expected) then $\text{VNIKX}(I,J)$ is filled with value of $(J-1)$ -st derivative of $N(\text{ILEFT}-K+I,K)$ at X , $I = 1, \dots, K$, $J = 1, \dots, \text{NDERIV}$. Get derivative from right or left if $X = T(\text{ILEFT})$ or $T(\text{ILEFT}+1)$, respectively. Expects NDERIV in $[1,K]$. Uses BSPLVN. Used in NATSPP.

subroutine INTERV(XT,LXT,X,ILEFT,MFLAG)

Computes largest ILEFT in $[1,LXT]$ such that $XT(\text{ILEFT}) \leq X$. It is assumed that XT is a one-dimensional array of length LXT containing a nondecreasing sequence of real numbers. The subroutine returns integers ILEFT and MFLAG as follows:

$$\text{if } \left\{ \begin{array}{l} X < XT(1) \\ XT(I) \leq X < XT(I+1) \\ XT(LXT) \leq X \end{array} \right\}, \text{ then } \left\{ \begin{array}{ll} \text{ILEFT} & \text{MFLAG} \\ 1 & -1 \\ I & 0 \\ LXT & 1 \end{array} \right.$$

The value of ILEFT is saved in a local variable IL0 which under certain conditions is used to start the search for ILEFT in the next call. The local variable IL0 is initialized to the value one.

Note that only BSPLPP, BSPLVN and BSPLVD are called directly by the natural spline interpolation subroutine NATSPP. In addition to these subroutines of the de Boor package, NATSPP also calls subroutines **BANDET** and **BANDSL** for the solution of the linear system $CX = B$ where C is an

unsymmetric band matrix. These subroutines were taken from the library of the Stanford Center for Information Processing. They are translations of ALGOL 60 procedures given by Martin and Wilkinson [LO]. They are fully described in the complete listing of the FORTRAN subroutines in Appendix I.

Turning now to the subroutine NATSPP for the interpolating natural spline we note that it is a direct implementation of the method described in Section 3. First we give a summary of the FORTRAN variables and their intended use. The heading of the subroutine is

```
SUBROUTINE NATSPP(N2,N3,N4,M,M2,MM,X,Y,A,C,T,Q,TRL,INT,VNIKX) .
```

The input parameters are as follows:

N2 , the number of data points.

N4 , = $N2 + M2 - 4$.

M , $2 * M - 1$ is the degree of the natural spline
admissible values range from 1 to N2 .

M2 , = $2 * M$, the order of the natural spline.

MM , = $2 * M - 1$, the degree of the natural spline.

X(1), ..., X(N2) , abscissas of the data points which must be strictly
monotone increasing.

Y(1), ..., Y(N2) , ordinates of the data points.

The output parameters are as follows:

N3 , = $N2 - 1 + MM$, the number of B-splines in the B-spline representation (1.2).

A(1), ..., A(N3) , the coefficients of the B-spline representation (1.2) of the
natural spline.

C(1,1), ..., C(M2,N2-1) , the coefficients of the piecewise polynomial
representation (1.1) of the natural spline.

The remainder of the parameters are only for temporary storage. They are included in the declaration in order to make it possible to give them variable dimensions. They are:

$T(1), \dots, T(N2+4*M-2)$, the knot sequence.

$Q(1,1), \dots, Q(N4, M2)$, elements of the band matrix of the equations for the calculation of the $A(1)$.

$TRL(1,1), \dots, TRL(N4, M-1)$, matrix for storing lower triangular matrix of the LU decomposition of the band matrix.

$INT(1), \dots, INT(N4)$, vector for recording row interchanges during decomposition of the band matrix.

$VNIKX(1,1), \dots, VNIKX(M2, MM)$, matrix for storing values and derivatives of B-splines as needed.

The subroutine NATSPP begins by computing the knot sequence $T(1)$ from the abscissas of the data points. In order to get the coefficients of the first $M-1$ rows of the band matrix which are given by (3.8) we call

$BSPLVD(T, M2, X(1), M2, VNIKX, MM)$

to obtain $VNIKX(I, J) = D^{J-1}_{N_I} (X(1))$, $I = 1, \dots, M2$, $J = 1, \dots, MM$. We use these to calculate $A(1)$ and the coefficients of the first $M-1$ rows and their right members. For the coefficients of the last $M-1$ rows of the band matrix which are given by (3.9) we call

$BSPLVD(T, M2, X(N2), N3, VNIKX, MM)$

to obtain $VNIKX(I, J) = D^{J-1}_{N_{N2-2+I, M2}} (X(N2))$, $I = 1, \dots, M2$, $J = 1, \dots, MM$. We use these to calculate $A(N2+2*M-2)$ and the coefficients of the last $M-1$ rows and their right members. For the coefficients of the rest of the rows of the band matrix which are given

by (3.6) (omitting first and last equations) we call

BSPLVN(T,M2,1,X(I),I+MM,VNIKX)

to obtain $VNIKX(J,1) = N_{I-1+J, M2}(X(I))$, $J = 1, \dots, M2$, $I = 2, \dots, N2-1$.

The band matrix system is then solved using BANDET and BANDSL to obtain the coefficients A(1) . Finally we call

BSPLPP(T, A, N3, M2, Q, X, C, LXI)

to calculate the derivatives needed to produce the coefficients of the piecewise polynomial representation. Note that in BSPLPP, $C(J,I)$ has the value $D^{J-1}S(X(I)^+)$ whereas in NATSPP, $C(J,I)$ has the value $D^{J-1}S(X(I)^+)/ (J-1)!$.

The complete listing of NATSPP with all embedded subroutines is given in Appendix I.

5. The ALGOL W Procedure.

Since we have available ALGOL W versions of the procedure **NATSPLINE** of Algorithm 472 of **Herriot** and **Reinsch** [8] and of Algorithm 480 of **Lyche** and **Schumaker** [9], it would be much easier to make comparison tests with the algorithm using the de Boor package [4] to calculate the interpolating natural spline if it were implemented in ALGOL W. The FORTRAN subroutine **NATSPP** was therefore translated into an ALGOL W procedure **DEBNAT**.

First the subroutines of the de Boor package used in **NATSPP** were translated into ALGOL W procedures with the same names and the same parameters. Special care was needed to deal with two unusual features of the FORTRAN package. In order to save the value of the local variable **IL0** of **INTERV** and of the local variable **J** in **BSPLVN** from one call to the next, these variables were made global to all the procedures of the de Boor package (**J** was renamed **JJ**). For the same reason the arrays **DELTAM** and **DELTAP** used in **BSPLVN** were made global. These global quantities were initialized prior to any calls of the package procedures. The other unusual feature of the FORTRAN subroutines was use of **VNIKX** as a one-dimensional array in **BSPLVN** and as a two-dimensional array in **BSPLVD**. This was handled by making **VNIKX** a two-dimensional array in **BSPLVD** and introducing a corresponding one-dimensional array **NVNIKX** local to **BSPLVD**,

The ALGOL W procedures **BANDET** and **BANSOL** are completely similar to the corresponding FORTRAN subroutines. They are fully described in the complete listing of the ALGOL W procedures in Appendix II.

Because of the greater flexibility of ALGOL W in using dynamic array declarations, it was possible to reduce the number of formal parameters

in the procedure DEBNAT compared to those in NATSPP. The heading of the procedure is

```
PROCEDURE DEBNAT(INTEGER VALUE N1,N2,M; REAL ARRAY X(*);
                 REAL ARRAY A(*,*); REAL ARRAY CFF(*));
```

The input parameters are as follows:

N1,N2 , subscript of first and last data point.

M , $2*M-1$ is the degree of the natural spline

admissible values range from 1 to $N2-N1+1$.

X(N1::N2) , contains the given abscissas X(1) which must be strictly monotone increasing.

A(N1::N2,0::2*M-1) , contains the given ordinates as zero-th column, i.e., A(I, 0) represents Y(I) .

The output parameters are as follows:

A(N1::N2,0::2*M-1) , the coefficients of the piecewise polynomial representation (1.1) of the natural spline with $c_{j,i} = A(i,j-1)$. (A(N2,0) is unchanged and no values are assigned to the last row of A .)

CFF(1::N2-N1+2*M-1) , the coefficients of the B-spline representation (1.2) of the natural spline.

The ALGOL W procedure DEBNAT is an exact translation of the FORTRAN subroutine NATSPP. The complete listing of DEBNAT with all embedded procedures is given in Appendix II.

Included among the tests described in Section 6 were tests to verify that NATSPP and DEBNAT produced the same results.

Another advantage of the ALGOL W procedure is that it is much easier to convert it to double precision arithmetic than it is to convert the FORTRAN subroutine NATSPP and the de Boor FORTRAN package to double precision arithmetic.

11. Tests.

Both the FORTRAN subroutine NATSPP and the ALGOL W procedure DEBNAT were tested extensively on the IBM 370/168 at the Stanford Center for Information Processing.

In order to verify that the routines were operating correctly for the evaluation of the polynomial coefficients of the spline $S(x)$, the values of $D^j S(x)/j!$, $j = 0, 1, \dots, 2m-2$ were calculated at the right-hand endpoint of each subinterval $[x_i, x_{i+1})$ and compared with their values (the coefficients in equation (1.1)) at the left-hand endpoint of the next subinterval. For the first test we used the five data points $(-3, 7)$, $(-1, 11)$, $(0, 26)$, $(3, 56)$, $(4, 29)$ with nonequidistant abscissas. Table I shows the results of a typical run using the FORTRAN subroutine NATSPP with $m = 2$ for these data points. The first line of each box gives the tabulated quantities at the given value of x which is the left-hand endpoint of the subinterval, and the second line of the box gives the tabulated quantities at the right-hand endpoint of the same subinterval. Similar results were obtained for $m = 1, 3, 4, 5$ for the same data points. The close agreement of these quantities $D^j S(x)/j!$, $j = 0, 1, \dots, 2m-2$ to the left and right of each breakpoint shows that the spline function and its derivatives satisfy the specified continuity conditions. This is a good indication of the correctness of the results. Note that in Table I $S''(-3)$ differs very slightly from its specified value of 0 and that $S(0)$ and $S(3)$ differ from their prescribed values in the least significant digit. Exactly the same results were obtained using the ALGOL W procedure DEBNAT. These results are very close to those obtained by using NATSPLINE which are given in Table I of Algorithm 472[8].

x	S(x)	S'(x)	S''(x)/2	S'''(x)/3!
-3.000000	7.000000 10.999999	-1.999995 9.999986	$-.4291534 \times 10^{-5}$ 5 . 1e-16 1e-16 1e-16	1.000000 1.000000
-1.000000	11.000000 25 . 1e-16 1e-16	9.999997 18.99998	6.000000 2 . 1e-16 1e-16 1e-16	-1.000001 -1.000001
0	25.99995 55 . 1e-16 1e-16 1e-16	18.99998 10 1e-16 1e-16 1e-16 1e-16	2.999995 -14 . 1e-16 1e-16 1e-16	-1.999998 -1.999998
3.000000	55.99998 29.00000	-16.99998 -32.00000	1e-16 1e-16 1e-16 1e-16 1e-16 $-.3242493 \times 10^{-4}$	4.999987 4.999987
4.000000	29.00000			

Table I. Cubic Natural Spline.

Five nonequidistant knots. Coefficients
calculated by NATSPP.

The same test was run for ten data points (x_i, y_i) with equidistant abscissas $x_i = i$ and ordinates given by

$$y_i = \left\{ \begin{array}{ll} 1 & , \quad i \text{ odd} \\ 0 & , \quad i \text{ even} \end{array} \right\} \quad i = 1, 2, \dots, 10 \quad . \quad (4.1)$$

For $m = 1, \dots, 5$ the FORTRAN subroutine NATSPP and the ALGOL W procedure DEBNAT gave the same results. In all cases the specified continuity conditions at the breakpoints were satisfied.

The previous tests established that the FORTRAN subroutine NATSPP and the ALGOL W procedure DEBNAT produced identical results. Further tests for accuracy and timing were carried out using only the ALGOL W procedure DEBNAT. Corresponding results for the accuracy of NATSPP can be inferred from these tests.

As a check on the correctness of the piecewise polynomial coefficients, long precision versions of DEBNAT and NATSPLINE from Algorithm 472[8] were used to calculate the polynomial coefficients for the data points $(-3, 7)$, $(-1, 11)$, $(0, 26)$, $(3, 56)$, $(4, 29)$ (data for Table I) for $m = 1, 2, \dots, 5$. When rounded to short precision, the corresponding coefficients calculated by the two procedures were identical, (Except that for $D^j S(1)/j!$, $j = m, \dots, 2m-2$, NATSPLINE gave the specified values 0 and DEBNAT gave values of order 10^{-t} , $t > 9$.) The same comparison test was run for the set of N_2 data points (x_i, y_i) with equidistant abscissas $x_i = i$ and ordinates given by

$$y_i = \left\{ \begin{array}{ll} 1 & , \quad i \text{ odd} \\ 0 & , \quad i \text{ even} \end{array} \right\} \quad i = 1, \dots, N_2 \quad . \quad (6.2)$$

Values of $N_2 = 10, 20, \dots, 50$ and $m = 1, 2, \dots, 7$ were used.' Again when the long precision coefficients were rounded to short precision, the corresponding coefficients calculated by the two procedures were identical (with the same exceptions as above and occasional differences in the least significant digit for the case $m = 7$).

In order to study the effect of round-off error build-up, both long and short precision versions of DEBNAT were used to calculate the B-spline coefficients and the piecewise polynomial coefficients. From the previous comparison tests we see that we can regard the long precision coefficients to be correct and hence the differences between the long precision and short precision coefficients are the errors in the latter. This error test was first run for the data points of Table I for $m = 1, 2, \dots, 5$. For $m = 1$ all short precision coefficients calculated by DEBNAT are exactly correct. For $m = 2$, the maximum errors in the B-spline coefficients and in the piecewise polynomial coefficients were of order approximately 10^{-5} . For $m = 3$ and 4 the maximum errors increased to about 10^{-3} . For $m = 5$ the errors exceeded one and the results were unacceptable. This may be due in part to the fact that for five points, $m = 5$ is an extreme case. Tests were also run for the example with equidistant knots and ordinates given by (6.2). Values of $N_2 = 10, 20, \dots, 50$ and $m = 1, 2, \dots, 7$ were used. The results for $m = 1, 2, 3, 4$ were similar to those for the data of Table I. For $m = 5$ the maximum errors were of order 10^{-2} . For $m = 6, 7$ the maximum errors exceeded one.

-Long precision and short precision versions of NATSPLINE were used on the same data to find the errors in the piecewise polynomial coefficients calculated by short precision NATSPLINE. The results appeared to be

somewhat better than for DEBNAT. For the data used in Table I, the maximum errors in the piecewise polynomial coefficients were 0 for $m = 1$ and of order 10^{-5} for $m = 2, \dots, 5$. For the example with equidistant knots and ordinates given by (6.2), the maximum errors in the piecewise polynomial coefficients were 0 for $m = 1$, of order 10^{-5} for $m = 2, 3$, of order 10^{-4} for $m = 4$, of order 10^{-2} for $m = 5$, and of order 10^{-1} for $m = 6, 7$.

We conclude that DEBNAT should not be used in short precision for $m > 5$ and NATSPLINE should not be used in short precision for $m \geq 7$.

In addition to the tests for accuracy, timing tests were carried out for long precision and short precision versions of both DEBNAT and NATSPLINE on the IBM 370/168 computer at the Stanford Center for Information Processing. The tests were made using the example with equidistant knots and ordinates given by (6.2). Values of $N_2 = 10, 20, \dots, 100$ and $m = 1, 2, \dots, 7$ were used. The time for both procedures was found to be approximately proportional to the number N_2 of knots. For DEBNAT the time was found to be approximately proportional to $m^{1.7}$ for $m \geq 3$ while for NATSPLINE it was approximately proportional to m^2 . The actual times were almost exactly the same for the short precision and long precision versions.

The time T in seconds for the execution of the procedure DEBNAT was found to be approximately

$$T = (N/60)(.0265m^{1.7}) , \quad m \geq 3 .$$

This formula seriously underestimates the time for $m = 1$ and 2 .

For NATSPLINE the time was found to be approximately

$$T = (N/60)(.015m^2) .$$

For $m < 5$ the times for NATSPLINE were somewhat less than those for DEBNAT, but for $m > \underline{6}$ the times were nearly the same.

Since we found that for the IBM 370/168 the times for short precision and long precision are nearly the same, we recommend the use of long precision for all calculations using these procedures. Converting the given ALGOL W procedures to long precision requires only replacement of all real identifiers by long real identifiers. The same recommendation would apply to any machine on which long precision is approximately as fast as short precision.

For reasons of accuracy we would also recommend the use of double precision for the FORTRAN subroutines. We have not attempted to convert the FORTRAN de Boor package to double precision.

References

1. Anselone, P. M. and Laurent, P. J., "A general method for the construction of interpolating and smoothing spline functions," Numer. Math. 12 (1968), 66-82.
2. de Boor, Carl, "On uniform approximation by splines," J. Approximation Theory 1 (1968), 219-235.
3. de Boor, Carl, "On calculating with B-splines," J. Approximation Theory 6 (1972), 50-62.
4. de Boor, Carl, "Package for calculating with B-splines," MRC Technical Summary Report #1333, Mathematics Research Center, The University of Wisconsin -Madison, Oct. 1973.
5. Curry, H. B. and Schoenberg, I. J., "On Pólya frequency functions. IV. The fundamental spline functions and their limits," J. Analyse Math. 17 (1966), 71-107.
6. Greville, T. N. E., "Spline functions, interpolation and numerical quadrature." In Mathematical Methods for Digital Computers, Vol. II. A. Ralston and H. S. Wilf (Eds.), Wiley, New York, 1967.
7. Greville, T. N. E., "Introduction to spline functions." In Theory and Applications of Spline Functions. T. N. E. Greville (Ed.), Academic Press, New York, 1969, pp. 1-35. (Pub. No. 22 Mathematics Research Center, U.S. Army, U. of Wisconsin.)
8. Herriot, John G. and Reinsch, Christian H., "Algorithm 472. Procedures for natural spline interpolation," Comm. ACM 16 (1973), 763-768.
9. Lyche, Tom and Schumaker, Larry L., "Algorithm 480. Procedures for computing smoothing and interpolating natural splines," Comm. ACM 17 (1974), 463-467.
10. Martin, R. S., and Wilkinson, J. H., "Solution of symmetric and unsymmetric band equations and the calculation of eigenvectors of band matrices," Numer. Math. 9 (1967), 279-301. Also in J. H. Wilkinson and C. Reinsch, Linear Algebra, Handbook for Automatic Computation, vol. II, F. L. Bauer (chief Ed.), Band 186 in die Grundlehren der mathematischen Wissenschaften, Springer-Verlag, New York, Heidelberg, Berlin. 1971, pp. 70-92.

APPENDIX I

```

1.      SUBROUTINE NATSPP(N2,N3,N4,M,M2,MM,X,Y,A,C,T,Q,TRL,INT,VNICKX)
2.      C      NATSPP COMPUTES THE COEFFICIENTS OF BOTH THE PIECEWISE
3.      C      POLYNOMIAL REPRESENTATION AND THE B-SPLINE REPRESENTATION OF A
4.      C      NATURAL SPLINE(X) OF DEGREE (2*M-1), INTERPOLATING THE
5.      C      ORDINATES Y(I) AT POINTS X(I), I=1 THROUGH N2.
6.      C      PIECEWISE POLYNOMIAL REPRESENTATION:
7.      C      FOR XX IN (X(1),X(I+1)), I=1,...,N2-1,
8.      C      S(XX)=C(1,I)+C(2,I)*T+...+C(2*M,I)*T**(2*M-1)
9.      C      WITH T=XX-X(I).
10.     C      B-SPLINE REPRESENTATION:
11.     C      FOR XX IN (X(1),X(N2)),
12.     C      S(XX)=A(1)*N(1,2*M,XX)+A(2)*N(2,2*M,XX)+...
13.     C      +A(N2+2*M-2)*N(N2+2*M-2,2*M,XX)
14.     C      WHERE N(J,2*M,XX) IS THE (NORMALIZED) B-SPLINE OF DEGREE
15.     C      (2*M-1) ON THE KNOT SEQUENCE T(J),...,T(J+2*M).
16.     C      INPUT:
17.     C      N2      THE NUMBER OF DATA POINTS
18.     C      N4      =N2+M2-4
19.     C      M       2*M-1 IS THE DEGREE OF THE NATURAL SPLINE,
20.     C      ADMISSIBLE VALUES RANGE FROM 1 TO N2,
21.     C      RECOMMENDED VALUES ARE NOT GREATER THAN 5 (SAY)
22.     C      M2      =2*M, THE ORDER OF THE NATURAL SPLINE
23.     C      MM      =2*M-1, THE DEGREE OF THE NATURAL SPLINE
24.     C      X(1),...,X(N2) ABSCISSAS OF THE DATA POINTS WHICH
25.     C      MUST BE STRICTLY MONOTONE INCREASING
26.     C      Y(1),...,Y(N2) ORDINATES OF THE DATA POINTS
27.     C      OUTPUT:
28.     C      N3      =N2-1+MM, THE NUMBER OF B-SPLINES IN THE
29.     C      B-SPLINE REPRESENTATION OF THE NATURAL SPLINE
30.     C      A(1),...,A(N3) THE COEFFICIENTS OF THE B-SPLINE
31.     C      REPRESENTATION OF THE NATURAL SPLINE
32.     C      C(1,1),...,C(M2,N2-1) THE COEFFICIENTS OF THE PIECEWISE
33.     C      POLYNOMIAL REPRESENTATION OF THE NATURAL SPLINE
34.     C      TEMPORARY STORAGE:
35.     C      T(1),...,T(N2+4*M-2) THE KNOT SEQUENCE
36.     C      Q(1,1),...,Q(N4,M2) ELEMENTS OF THE BAND MATRIX OF THE
37.     C      EQUATIONS FOR THE CALCULATION OF THE A(I)
38.     C      TRL(1,1),...,TRL(N4,M-1) MATRIX FOR STORING LOWER-TRIANGULAR
39.     C      MATRIX OF THE LU DECOMPOSITION OF THE BAND MATRIX
40.     C      INT(1),...,INT(N4) VECTOR FOR RECORDING ROW INTERCHANGES
41.     C      DURING DECOMPOSITION OF THE BAND MATRIX
42.     C      VNICKX(1,1),...,VNICKX(M2,MM) MATRIX FOR STORING VALUES AND
43.     C      DERIVATIVES OF B-SPLINES AS NEEDED
44.     C      DIMENSION X(1),Y(1),T(1),Q(N4,1),A(1),VNICKX(M2,MM),TRL(N4,1),
45.     C      1 INT(1),C(M2,1)
46.     C      DO 5 I=1,MM
47.     C      5 T(I)=X(1)
48.     C      N2M1=N2-1
49.     C      DO 6 I=1,N2M1
50.     C      6 T(I+MM)=X(I)
51.     C      N3=N2M1+MM
52.     C      DO 7 I=1,M2
53.     C      7 T(I+N3)=X(N2)
54.     C      GET COEFFICIENTS OF FIRST M-1 ROWS
55.     C      CALL BSPLVD(T,M2,X(1),M2,VNICKX,MM)
56.     C      A1=Y(1)/VNICKX(1,1)
57.     C      MM1=M-1
58.     C      IF (M.EQ.1) GO TO 70
59.     C      DO 40 I=1,MM1
60.     C      DO 41 J=1,MM

```

```

61.      41      Q(I,J)=0.
62.      HP I=M+I
63.      LL=M-I
64.      DO 42 L=2,MPI
65.          LL=LL+1
66.      42      Q(I,LL)=VNIKX(L,HP I)
67.      40      A(I)=-A1*VNIKX(L,MPI)
68. C      GET COEFFICIENTS OF NEXT N2-2 ROWS
69.      70 MM2=M-2
73.      DO 30 I=2,N2M1
71.          CALL BSPLVN(T,M2,I,X(I),I+MM,VNIKX)
72.          IM2=I+MM2
73.          DO 16 L=1,MM
74.              16      Q(IM2,L)=VNIKX(L,IJ
75.      30      A(IM2)=Y(I)
76. C      GET COEFFICIENTS OF LAST H-A ROWS
77.          CALL BSPLVD(T,M2,X(N2),N3,VNIKX,MM)
78.          ANP=Y(N2)/VNIKX(M2,1)
79.          IF (M.EQ.1) GO TO 80
80.          DO 50 I=1,MM1
81.              II=N2+M2-3-I
82.              DO 51 J=1,MM
83.                  51      Q(II,J)=0.
84.              MPI=M+I
85.              MPI M1=MPI - 1
86.              LL=M-I
87.              DO 52 L=1,MPI M1
88.                  LL=LL+1
89.                  52      Q(II,L)=VNIKX(LL,MPI)
90.              50      A(II)=-ANP*VNIKX(M2,MPI)
91.      80 CONTINUE
92.          CALL BANDET(TRL,INT,Q,N4,M-1,2*M-1)
93.          CALL BANDSL(TRL,INT,A,Q,N4,M-1,2*M-1)
94.          DO 60 I=1,N4
95.              J=N3-I
96.      60      A(J)=A(J-1)
97.      A(1)=A1
98.      A(N3)=ANP
99.      CALL BSPLPP(T,A,N3,M2,J,X,C,LXI)
100.      DO 12 I=1,N2M1
101.          FAC=1.0
102.          DO 12 J=2,M2
103.              FJ=FLOAT(J-1)
104.              FAC=FAC*FJ
105.      12      C(J,I)=C(J,I)/FAC
106.      RETURN
107.      END
108. C      ***** STAR J OF BANDET *****
109. C      PRIOR TO 03/23/72
110. C      BANDET AND BANDSL ARE TWO SUBROUTINES WHICH SOLVE C*X = B
111. C      WHEN C IS AN UNSYMMETRIC BAND MATRIX (THEY WILL WORK WITH
112. C      SYMMETRIC BAND MATRICES BUT TAKE NO ADVANTAGE OF THEIR
113. C      STRUCTURE).
114. C
115. C      C HAS M1 SUBDIAGONALS AND M2 SUPERDIAGONALS.
116. C      THE MATRIX C IS TRANSFORMED TO A BY MAKING EACH DIAGONAL OF
117. C      C A COLUMN OF A. THUS A IS NX(M1+M2+1) WHEN C IS NXN.
118. C      A TYPICAL A IS PICTURED BELOW. C HERE IS 4X4, WITH
119. C      2 SUBDIAGONALS AND 1 SUPERDIAGONAL
120. C
121. C      0          0          C(1,1)          C(1,2)

```

```

122.      C      0      C(2,1)      C(2,2)      C(2,3)
123.      c      C(3,1)      C(3,2)      C(3,3)      C(3,4)
124.      C      C(4,2)      C(4,3)      C(4,4)      0
125.      C
126.      C      THIS TRANSFORMATION IS THE FOLLOWING, ASSUMING THAT C (I ,J)
127.      C      IS A BAND ELEMENT IN C:
128.      C      C(I,J) --> A(I,M1+1+(J-1))
129.      C      ALL OTHER ELEMENTS OF A ARE 0
130.      C
131.      C      BANDET FINDS THE LU DECOMPOSITION OF A , STORING
132.      C      THE LOWER TRIANGULAR MATRIX IN M AND NXM1 MATRIX,
133.      C      AND OVERWRITING THE UPPER TRIANGULAR MATRIX INTO A .
134.      C      BANDSL USES THIS DECOMPOSITION TO SOLVE A*X = B WHERE
135.      C      THE RIGHTHAND SIDE IS INPUT IN THE VECTOR B, AND X IS
136.      C      OUTPUT IN THE VECTOR B.
137.      C
138.      C      THESE ROUTINES WERE TRANSLATED FROM THOSE PRESENTED BY
139.      C      J. WILKINSON IN NUMERISCHE MATHEMATIK VOL 9, P 283
140.      C      TRANSLATOR: BARBARA RYDER, CSD SERRA HOUSE, X3124
141.      C
142.      C      SUBROUTINE BANDET(M,INT,A,N,M1,M3)
143.      C      DIMENSION M(N,M1),INT(N),A(N,M3)
144.      C
145.      C      M-----AN NXM1 MATRIX FOR STORING LOWER TRIANGULAR
146.      C      MATRIX OF LU DECOMPOSITION OF A
147.      C      INT---A NNX1 VECTOR FOR RECORDING ROW INTERCHANGES
148.      C      DURING DECOMPOSITION
149.      C      A-----AN NX(M1+M2+1) MATRIX WHOSE COLUMNS ARE THE DIAGONALS
150.      C      OF C, THE BAND MATRIX BEING DECOMPOSED
151.      C      A(*,1) - A(*,M1) ARE SUBDIAGONALS OF C
152.      C      A(*,M1+1) ARE SUBDIAGONALS OF C
153.      C      A(*,M1+2) - A(*,M1+M2+1) ARE SUPERDIAGONALS OF C
154.      C      N----NUMBER OF ROWS IN A
155.      C      M1----NUMBER OF SUBDIAGONALS IN C
156.      C      M3----TOTAL NUMBER OF DIAGONALS IN C, I.E. WIDTH OF BAND
157.      C      M3 = M1 (# SUBDIAGS) + M2 (# SUPERDIAGS) + 1
158.      C
159.      C      REAL M
160.      25      L=M1
161.      C      DO 40 I=1,M1
162.      C      K2=M1+2-I
163.      C      DO 50 J=K2,M3
164.      50      A(I,J-L)=A(I,J)
165.      C      L=L-1
166.      C      K2=M3-L
167.      C      DO 60 J=K2,M3
168.      C      A(I,J)=0.0
169.      40      CONTINUE
170.      45      L=M1
171.      C      DO 70 K=1,N
172.      C      X=A(K,1)
173.      C      I=K
174.      C      K2=K+1
175.      C      IF (L.LT.N) L=L+1
176.      72      IF (L.LT.K2) GO TO 81
177.      79      DO 80 J=K2,L
178.      C      IF (ABS(A(J,1))-ABS(X)) 80,80,82
179.      82      X=A(J,1)
180.      C      I=J
181.      80      CONTINUE
182.      81      INT(K)=I

```

```

183.      I F(X) 73,75,73
184.      73 IF (I-K) 77,78,77
185.      77 DO 9 0 J=1,M3
186.      X=A(K,J)
187.      A(K,J)=A(I,JJ)
188.      90 A(I,J)=X
189.      78 I F(L.LT.K2) G O T J 70
193.      83 DO 100 J=K2,L
191.      M(K,J-K)=A(J,I)/A(K,I)
192.      X=M(K,J-K)
193.      DO 110 JJ=2,M3
194.      110 A(J,JJ-1)=A(J,JJ)-A(K,JJ)*X
195.      100 A(J,M3)=0.0
196.      70 CONTINUE
197.      RETURN
198.      C
199.      C A SUBROUTINE CALLED ERRJRMUSTBE SUPPLIED TO HANDLE
200.      C THE ZERO PIVOT SITUATION; 4 SAMPLE ROUTINE FOLLOWS
201.      C
202.      75 CALL ERROR
203.      RETURN
204.      END
205.      SUBROUTINE ERRCK
206.      200 FORMAT(//' ZERO PIVOT')
207.      WRITE(6,200)
208.      RETURN
209.      END
210.      C ***** END OF BANDET *****
211.      C ***** START OF BANDSL *****
212.      C PRIOR TO 3/23/72
213.      SUBROUTINE BANDSL (M,INT,B,A,N,M1,M3)
214.      DIMENSION INT(N),A(N,M3),M(N,M1),B(N)
215.      C
216.      C ALL PARAMETERS SAME AS IN BANDET EXCEPT FOR:
217.      C B-----RIGHTHAND SIDE OF LINEAR SYSTEM C*X = B
218.      C SOLUTION IS RETURNED IN B
219.      C
220.      REAL M
221.      INTEGER W
222.      L=M1
223.      DO 10 K=1,N
224.      I=INT(K)
225.      IF (1-K) 11,12,11
226.      11 X=B(K)
227.      B(K)=B(I)
228.      B(I)=X
229.      12 K2=K+1
230.      IF (L.LT.N) L=L+1
231.      14 IF (L.LT.K2) G O T O 1 3
232.      15 DO 2 0 I=K2,L
233.      X=M(K,I-K)
234.      20 B(I)=B(I)-X*B(K)
235.      10 CONTINUE
236.      L=1
237.      DO 30 I=1,N
238.      I=N+1-I
239.      X=B(I)
240.      W= I-1
241.      I F(L-1) 32,33,32
242.      32 DO C 0 K=2,L
243.      40 X=X-A(I,K)*B(K+W)

```

```

244.      33      B(I)=X/A(I,1)
245.          I F (L-M3) 31,30,30
246.      31      L=L+1
247.      30      CONTINUE
248.          RETURN
249.          END
253.  C ***** END OF BANDSL *****
251.          SUBROUTINE BSPLDR(T,A,N,K,ADIF,NDERIV)
252.  CONSTRUCTS DIV.DIFF.TABLE FOR B-SPLINE COEFF. PREPARATORY TO DERIV.CALC.
253.          DIMENSION T(1),A(1),ADIF(N,NDERIV)
254.          DO 10 I=1,N
255.      LO      ADIF(I,1) = A(I)
256.          KMID = K
257.          DO 20 ID=2,NDERIV
258.              KMIO = KMID - 1
259.              FKHI0 = FLOAT(KMID)
260.              DO 20 I=ID,N
261.                  IPKMID = I + KMID
262.                  DIFF = T(IPKMID) - T(I)
263.                  I F (DIFF .EQ. 0.)          GO TO 20
264.                  ADIF(I,ID) = (ADIF(I,ID-1) - ADIF(I-1, ID-1))/DIFF*FKMID
245.      20      CONTINUE
266.                      RETURN
267.          END
268.          SUBROUTINE BSPLEV(T,ADIF,N,K,X,SVALUE,NDERIV)
269.  CALCULATES VALUE OF SPLINE AND ITS DERIVATIVES AT *X* FROM B-REPR.
270.          DIMENSION T(1),ADIF(N,NDERIV),SVALUE(1)
271.          DIMENSION VNIKX(20)
272.          DO 5 IDUMMY=1,NDERIV
273.      S      SVALUE(IDUMMY) = 0
274.          KM1 = K-1
275.          CALL INTERV(T(K),N+1-<41,X,I,MFLAG)
276.          I = I+KM1
277.          IF (MFLAG)          GO TO 9
278.      9      I F (X .GT. T(I))          GO TO 9
279.      10     IF (I .EQ. K)          GO TO 99
280.          I = I - 1
281.          I F (X .EQ. T(I))          GO TO 10
282.  C
283.  C *I* HAS BEEN FOUND IN (K,N) SUCH THAT T(I) .LE. X .LT. T(I+1)
284.  C      ( O R .LE. T(I+1), I F T(I) .LT. T(I+1) = T(N+1) ).
285.      20     KP1MN = K+1-NDERIV
286.          CALL BSPLVN(T,KP1MN,1,X,1,VNIKX)
287.          IO = NDERIV
288.      21     LEFT = I - KP1MN
289.          DO 22 L=1,KP1MN
290.              LEFTPL = LEFT+L
291.      22     SVALUE(ID) = VNIKX(L)*ADIF(LEFTPL,ID) + SVALUE(ID)
292.          ID = IO - 1
293.          I F (ID .EQ. 0)          GO TO 99
294.          KP1MN = KP1MN + 1
295.          CALL BSPLVN(T,0,2,X,1,VNIKX)
296.                      GO TO 21
297.  C
298.      99      RETURN
299.          END
300.          SUBROUTINE BSPLPP(T,A,N,K,SCRATCH,XI,C,LXI)
301.  CONVERTS B-SPLINE REPRESENTATION TO PIECEWISE POLYNOMIAL REPRESENTATION
302.          DIMENSION T(1),A(1),SCRATCH(N,K),XI(1),C(K,1)
303.          CALL BSPLDR(T,A,N,K,SCRATCH,K)
304.          LXI = 0

```



```

305.      XI(1) = T(K)
306.      DO 5 0 ILEFT=K,N
307.          I F (T(ILEFT+1) .EQ. T(ILEFT))      ii3 TU 50
308.          LXI = LXI + 1
309.          XI(LXI+1) = T(ILEFT+1)
310.          CALL BSPLEV(T,SCRICH,N,K,XI(LXI),C(1,LXI),K)
311.      so      CONTINUE
312.  C
313.                      At TURN
314.      END
315.      SUBROUTINE BSPLVD ( T, C, X, ILEFT, VNIKX, NDERIV, J
316.      CALCULATES VALUE AND DERIV. OF ALL B-SPLINES WHICH DO NOT VANISH AT x
317.      DIMENSION T(1),VNIKX(K,NDERIV)
318.      DIMENSION A(20,20)
319.  C
320.  C F I L L VNIKX(J, IDERIV), J=IDERIV, ... ,K WITH NONZERO VALUES OF
321.  C B-SPLINES OF ORDER K+1-IDERIV, IDERIV=NDERIV, . . . , BY REPEATED
322.  C CALLS TO BSPLVN
323.      CALL BSPLVN(T,K+1-IDERIV,1,X,ILEFT,VNIKX(NDERIV,NDERIV))
324.      IF (NDERIV .LE. 1)      GO TO 99
325.      IDERIV = NDERIV
326.      0 0 1 5 I=2, NDERIV
327.      IDERVM = IDERIV-A
328.      DO 11 J=IDERIV,K
329.          11      V h f KX(J-I, IDERVM) = VNIKX(J, IDERIV)
330.          IDERIV = IDERVM
331.          CALL BSPLVN(T,0,2,X,ILEFT,VNIKX(IDERIV, IDERIV))
332.          15      CONTINUE
333.  C
334.      DO 20 I=1,K
335.          DO 1 9 J=1,K
336.              19      A(I,J) = 0
337.              20      A(I,I) = 1.
338.      KMD = K
339.      DO 40 M=2, NDERIV
340.          KMD = KMD-1
341.          FKMD = FLOAT(KMD)
342.          I = ILEFT
343.          J = K
344.          21      JMI = J - I
345.          IPKMD = I + KMD
346.          DIFF = T(IPKMD) - T(I)
347.          IF (JMI .EQ. 0)      GO TO L b
348.          I F (DIFF .EQ. 0.)      GO TO 25
349.          0 0 2 4 L=1, J
350.          24      A(L,J) = (A(L,J) - A(L,J-1))/DIFF*FKMD
351.          2s      J = JMI
352.          I = I - 1
353.                      GO TO CA
354.          26      IF (DIFF .EQ. 0.)      GO TO 30
355.          A(I,I) = A(I,I)/DIFF*FKMD
356.  C
357.      30      DO 4 0 I=1,K
358.          v = 0.
359.          JLOW = MAX0(I,M)
360.          DO 3 5 J=JLOW,K
361.              3 5      v = A(I,J)*VNIKX(J,M) + v
362.              40      VNIKX(I,M) = v
363.              99
364.          END
365.      SUBROUTINE BSPLVN(T,JHIGH,INDEX,X,ILEFT,VNIKX)

```

```

366.      CALCULATES THE VALUE OF ALL POSSIBLY NONZERO B-SPLINES AT *X* OF
367.      C O R D E R M A X ( J H I G H , ( J + 1 ) ( I N D E X - 1 ) ) O N * T *.
368.          D I M E N S I O N T ( 1 ) , V N I K X ( 1 )
369.          D I M E N S I O N D E L T A M ( 2 0 ) , D E L T A P ( 2 0 )
373.          D A T A J / 1 / , D E L T A M , D E L T A P / 4 0 * J . /
311.
372.      10 J = 1
373.          V N I K X ( 1 ) = 1
374.          I F ( J . G E . J H I G H )
375.      C
376.      20 I P J = I L E F T + J
377.          D E L T A P ( J ) = T ( I P J ) - X
378.          I M J P 1 = I L E F T - J + 1
379.          D E L T A M ( J ) = X - T ( I M J P 1 )
380.          V M P R E V = 0 .
381.          J P 1 = J + 1
382.          D O 2 6 L = 1 , J
383.              J P 1 M L = J P 1 - C
384.              V M = V N I K X ( L ) / ( D E L T A P ( L ) + D E L T A M ( J P 1 M L ) )
385.              V N I K X ( L ) = V M * D E L T A P ( L ) + V M P R E V
386.      26 V M P R E V = V M * D E L T A M ( J P 1 M L )
387.          V N I K X ( J P 1 ) = V M P R E V
388.          J = J P 1
389.          I F ( J . L T . J H I G H )
390.      C
391.      99
392.          E N D
393.          S U B R O U T I N E I N T E R V ( X T , L X T , X , I L E F T , M F L A G J
399.      C O M P U T E S L A R G E S T I L E F T I N ( 1 , L X T ) S U C H T H A T X T ( I L E F T ) . L E . X
395.          D I M E N S I O N X T ( L X T )
396.          D A T A I L O / 1 /
397.          I H I = I L O + 1
398.          I F ( I H I . L T . L X T )
399.              I F ( X . G E . X T ( L X T ) )
403.              I F ( L X T . L E . 1 )
401.              I L O = L X T - 1
402.
403.      2 0 I F ( X . G E . X T ( I H I ) )
404.      2 1 I F ( X . G E . X T ( I L O ) )
405.      C * * * * N O W X . L T . X T ( I H I ) . F I N D L O W E R B O U N D
406.      3 0 I S T E P = 1
407.      31 I H I = I L O
408.          I L O = I H I - I S T E P
409.          I F ( I L O . L E . 1 )
410.          I F ( X . G E . X T ( I L O ) )
411.          I S T E P = I S T E P * 2
412.
413.      35 I L O = 1
414.          I F ( X . L T . X T ( 1 ) )
415.
416.      C * * * * N O W X . G E . X T ( I L O ) . F I N D U P P E R B O U N D
417.      4 0 I S T E P = 1
418.      4 1 I L O = I H I
419.          I H I = I L O + I S T E P
423.          I F ( I H I . G E . L X T )
421.          I F ( X . L T . X T ( I H I ) )
422.          I S T E P = I S T E P * 2
423.
424.      45 I F ( X . G E . X T ( L X T ) )
425.          I H I = L X T
426.      C * * * * N O W X T ( I L O ) . L E . X . L T . X T ( I H I ) . N A K K R O N T H E I N T E R V A L

```

```

427.      5 0 MIDDLE = (ILO + IHI)/2
428.      I f (MIDDLE .EQ. ILO)      GO TO 100
429. C      NOTE. I TIS ASSUMED THAT MIDDLE = ILO IN CASE IHI = ILO+1
433.      I F (X .LT. XT(MIDDLE))    GO TO 5 3
431.      ILO = MIDDLE
432.      GO TO 50
433.      53 IHI = MIDDLE
434.      GO TO 50
435. C**** SET OUTPUT AND RETURN
436.      90 HFLAG = -1
437.      ILEFT = 1
438.      RETURN
439.      1 0 0 MFLAG = 0
440.      ILEFT = ILO
441.      RETURN
442.      110 HFLAG = 1
443.      ILEFT = LXT
444.      RETURN
445.      END

```

APPENDIX II

```

1.  PROCEDURE DEBNAT( INTEGER VALUE N1,N2,M; REAL A R R A Y X(*);
2.      REAL ARRAY A(*,*); REAL ARRAY CFF(*));
3.  COMMENT DEBNAT COMPUTES THE COEFFICIENTS OF BOTH THE PIECEWISE
4.      POLYNOMIAL REPRESENTATION AND THE B-SPLINE REPRESENTATION OF A
5.      NATURAL SPLINE S(X) OF DEGREE (2*M-1), INTERPOLATING THE
6.      ORDINATES Y(I) AT POINTS X(I), I=N1 THROUGH N2.
7.      PIECEWISE POLYNOMIAL REPRESENTATION:
8.      FOR XX IN (X(I), X(I+1)), I=N1, ..., N2-1,
9.      S(XX)=A(I,0)+A(I,1)*T+...+A(I,2*M-1)*T**(2*M-1)
13.     WITH T=XX-X(I).
11.     B-SPLINE REPRESENTATION:
12.     FOR XX IN (X(N1), X(N2)),
13.     S(XX)=CFF(1)*N(1,2*M,XX)+CFF(2)*N(2,2*M,XX)+...
14.           +CFF(N2-N1+2*M-1)*N(N2-N1+2*M-1,2*M,XX)
15.     WHERE N(J,2*M,XX) IS THE (NORMALIZED) B-SPLINE OF DEGREE
16.     (2*M-1) ON THE KNOT SEQUENCE T(J), ..., T(J+2*M).
17.     INPUT:
18.     N1,N2 SUBSCRIPT OF FIRST AND LAST DATA POINT
19.     M      2*M-1 IS THE DEGREE OF THE NATURAL SPLINE,
23.     ADMISSIBLE VALUES RANGE FROM 1 TO N2-N1+1,
21.     RECOMMENDED VALUES ARE NOT GREATER THAN 7 (SAY)
22.     X(N1::N2) CONTAINS THE GIVEN ABSCISSAS X(I) WHICH
23.     MUST BE STRICTLY MONOTONE INCREASING
24.     A(N1::N2,0::2*M-1) CONTAINS THE GIVEN ORDINATES A SZERO-TH
25.     COLUMN, I.E. A(I,0) REPRESENTS Y(I),
25.     OUTPUT:
27.     A(N1::N2,0::2*M-1) THE COEFFICIENTS OF THE PIECEWISE POLYNOMIAL
28.     REPRESENTATION OF THE NATURAL SPLINE, (A(N2,0) IS
29.     UNCHANGED AND NO VALUES ARE ASSIGNED TO THE LAST
30.     ROW OF A)
31.     CFF(1::N2-N1+2*M-1) THE COEFFICIENTS OF THE B-SPLINE
32.     REPRESENTATION OF THE NATURAL SPLINE;
33.     IF (M > 0) AND (M <= N2-N1+1) THEN
34.     BEGIN
35.     PROCEDURE BSPLDR(REAL ARRAY T,A(*); INTEGER VALUE N,K;
36.         REAL ARRAY ADIF(*,*); INTEGER VALUE NDERIV);
37.     COMMENT CONSTRUCTS DIV.DIFF. TABLE FOR B-SPLINE COEFF.
38.     PREPARATORY TO DERIV.CALC.. ARRAY DIMENSIONS ARE AS
39.     FOLLOWS: T(1::N+K), A(1::N), ADIF(1::N,1::NDERIV).
40.     NDERIV SHOULD BE IN (2,K);
41.     BEGIN
42.     INTEGER KMID;
43.     REAL DIFF;
44.     FOR I:=1 UNTIL N DO ADIF(I,1):=A(I);
45.     KMID:=K;
46.     FOR ID:=2 UNTIL NDERIV DO
47.     BEGIN
48.     KMID:=KMID-1;
49.     FOR I:=ID UNTIL N DO
53.     BEGIN
51.     DIFF:=T(I+KMID) - T(I);
52.     IF DIFF/=0 THEN
53.     ADIF(I, ID):=(ADIF(I, ID-1) - ADIF(I-1, ID-1))/DIFF*KMID
54.     END
55.     END
56.     END BSPLDR;
57.     PROCEDURE BSPLEV(REAL ARRAY T(*); REAL ARRAY ADIF(*,*);
58.         INTEGER VALUE N,K; REAL VALUE X;
59.         REAL ARRAY SVALUE(*); INTEGER VALUE NDERIV);
60.     COMMENT CALCULATES VALUE OF SPLINE AND ITS DERIVATIVES AT X FROM

```

```

61.          B-REPRESENTATION.  A&RAY DIMENSIONS ARE AS FOLLOWS:
62.          T(1::N+K), ADIF(1::N,1::NDERIV), SVALUE(1::NDERIV);
63.      BEGIN
64.          REAL ARRAY VNIKX(1::K);
65.          REAL ARRAY TT(1::N+1);
66.          INJEGER KM1,MFLAG,I,LEFT,ID,KP1MN;
67.          FOR I DUMMY:=1 UNTIL NDERIV DO SVALUE(IDJMMY) :=0;
68.          KM1:=K-1;
69.          FOR I DUMMY:=1 UNTIL N+1 DO TT(IDJMMY):=T(IDJMMY+K-1);
70.          INTERV(TT,N+1-KM1,X,I,MFLAG);
71.          I:=I+KM1;
72.          IF MFLAG<0 THEN GO TO S99
73.          ELSE IF MFLAG=0 THEN GO TO S20;
74.          IF X>T(I) THEN GO TO S99;
75.      S10:  IF I=K THEN GO TO S99;
76.          I:=I-1;
77.          IF X=T(I) THEN GO TO S10;
78.          COMMENT I HAS BEEN FOUND A N(K,N) S O THAT T(I)<=X<=T(I+1)
79.          (OR <=T(I+1), IF T(I)<T(I+1)=T(N+1));
80.      S20:  KP1MN:=K+1-NDERIV;
81.          BSPLVN(T,KP1MN,1,X,I,VNIKX);
82.          ID:=NDERIV;
83.      S21:  LEFT:=I-KP1MN;
84.          FOR L:=1 UNTIL KP1MND0
85.              SVALUE(ID):=VNIKX(L)*ADIF(LEFT+L,ID) + SVALUE(ID);
86.          ID:=ID-1;
87.          IF ID=0 THEN GO TO 393;
88.          KP1MN:=KP1MN+1;
89.          BSPLVN(T,0,2,X,I,VNIKX);
90.          GO TO S21;
91.      s99 :
92.          END BSPLVN;
93.          PROCEDURE BSPLPP(REAL ARRAY T,A(*);INTEGER VALUE N,K;
94.              REAL ARRAY SCRTCH(*,*);REAL ARRAY XI(*);
95.              REAL ARRAY C(*,*); INTEGER RESULT LXI);
96.          COMMENT CONVERTS B- SPLINE REPRESENTATION TO PIECEWISE POLYNOMIAL
97.          REPRESENTATION.  ARRAY DIMENSIONS ARE AS FOLLOWS:
98.          T(1::N+K), A(1::N), SCRTCH(1::N,1::K), XI(1::LXI+1),
99.          C(1::K,1::LXI).  LXI=N-K-1 IF NO REPEATED KNOTS;
100.      BEGIN
101.          BSPLDR(T,A,N,K,SCRTCH,K);
102.          LXI:=0;
103.          XI(1):=T(K);
104.          FOR ILEFJ:=K UNTIL N DO
105.              IF T(ILEFJ+1)~=T(ILEFJ) THEN
106.                  BEGIN
107.                      LXI:=LXI+1;
108.                      XI(LXI+1):=T(ILEFJ+1);
109.                      BSPLVN(T,SCRTCH,N,K,XI(LXI),C(*,LXI),K)
110.                  END
111.          END BSPLPP;
112.          PROCEDURE BSPLVN(REAL ARRAY T(*);INTEGER VALUE JHIGH,INDEX;
113.              REAL VALUE X;INTEGER VALUE ILEFJ;
114.              REAL ARRAY VNIKX(*));
115.          COMMENT CALCULATES THE VALUE OF ALL POSSIBLY NONZERO B-SPLINES AT X
116.          OF ORDER MAX(JHIGH,(JJ+1))(INDEX=1 JJ UNT.  INDEX=1 OR 2.
117.          J J , DELTAM, DELTAP ARE GLOBAL VARIABLES.
118.          BEFORE THE FIRST CALL ONE MUST SET JJ=1 AND ALL ELEMENT'S OF
119.          DELTAM AND DELTAP = 40.  ARRAY DIMENSIONS ARE AS FOLLOWS:
120.          T(1::N+K), VNIKX(1::K), DELTAM(1::K), DELTAP(1::K);
121.      BEGIN

```

```

122.      INTEGER JP1,JP1ML;
123.      REAL VMPREV,VM;
124.      IF INDEX=1 THEN
125.      BEGIN
126.          JJ:=1;
127.          VNIKX(1):=1;
128.          IF JJ>=JHIGH THEN GO TO S99
129.      END;
130. S20:  DELTAP(JJ):=T(ILEFT+JJ)-X;
131.      DELTAM(JJ):=X-T(ILEFT-JJ+1);
132.      VMPREV:=0;
133.      JP1:=JJ+1;
134.      FOR L:=1 UNTIL J-JDU
135.      BEGIN
136.          JP1ML:=JP1-L;
137.          VM:=VNIKX(L)/(DELTAP(L)+DELTAM(JP1ML));
138.          VNIKX(L):=VM*DELTAP(L)+VMPREV;
139.          VMPREV:=VM*DELTAM(JP1ML)
140.      END;
141.      VNIKX(JP1):=VMPREV;
142.      JJ:=JP1;
143.      IF JJ<JHIGH THEN GOTOS20;
144. S99:  ENDBSPLVN;
145.      PROCEDURE BSPLVN(REAL ARRAY T(*); INTEGER VALUE K;
146.          REAL VALUE X; INTEGER VALUE ILEFT;
147.          REAL ARRAY VNIKX(*, *); INTEGER VALUE NDERIV);
148.      COMMENT CALCULATES VALUE AND DERIVS. OF ALL B-SPLINES WHICH DO
149.      NOT VANISH AT X. ARRAY DIMENSIONS ARE AS FOLLOWS:
150.          T(1::N+K), VNIKX(1::K,1::NDERIV);
151.      BEGIN
152.          INTEGER IDERIV,IDERVM,KMD,I,J,JM1,JLW;
153.          REAL V,DIFF;
154.          REAL ARRAY NVNIKX(1::K);
155.          REAL ARRAY A(1::K,1::K);
156.          COMMENT FILL VNIKX(J,IDERIV), J=IDERIV,...,K WITH NONZERO
157.          VALUES OF B-SPLINES OF ORDER K+1-IDERIV,
158.          IDERIV=NDERIV,...,1 BY REPEATED CALLS TO BSPLVN;
159.          BSPLVN(T,K+1-NDERIV,1,X,ILEFT,NVNIKX);
160.          FOR IDUMMY:=NDERIV UNTIL K DO
161.              VNIKX(IDUMMY,NDERIV):=NVNIKX(IDUMMY-NDERIV+1);
162.          IF NDERIV<=1 THEN GOTOS99;
163.          IDERIV:=NDERIV;
164.          FOR I:=2 UNTIL NDERIV DO
165.          BEGIN
166.              IDERVM:=IDERIV-1;
167.              FOR J:=IDERIV UNTIL K DO
168.                  VNIKX(J-1,IDERVM):=VNIKX(J,IDERIV);
169.              IDERIV:=IDERVM;
170.              BSPLVN(T,0,2,X,ILEFT,NVNIKX);
171.              FOR IDUMMY:=IDERIV UNTIL K DO
172.                  VNIKX(IDUMMY,IDERIV):=NVNIKX(IDUMMY-IDERIV+1)
173.          END;
174.          FOR I:=1 UNTIL K DO
175.          BEGIN
176.              FOR J:=1 UNTIL K DO
177.                  A(I,J):=0;
178.              A(I,1):=1
179.          END;
180.          KMO:=K;
181.          FORM:=2 UNTIL NDERIV DO
182.

```

```

366.      CALCULATES THE VALUE OF ALL POSSIBLY NONZERO B-SPLINES AT *X* OF
367.      C O R D E R MAX(JHIGH,(J+1)(INDEX-1)) ON *T*.
368.      DIMENSION T(1),VNIKX(1)
369.      DIMENSION DELTAM(20),DELTAP(20)
373.      DATA J/1/,DELTAM,DELTAP/40*J./
371.                                         GO TO (10,20),INDEX
372.      10  J = 1
373.      VNIKX(1) = 1
374.      I F (J .GE. JHIGH)                GO TO 99
375. C
376.      20  IPJ = ILEFT+J
377.      DELTAP(J) = T(IPJ) - X
378.      IMJP1 = ILEFT-J+1
379.      DELTAM(J) = X - T(IMJP1)
380.      VMPREV = 0.
381.      JP1 = J+1
382.      DO 2 6 L=1,J
383.      JP1ML = JP1 - L
384.      VM = VNIKX(L)/(DELTAP(L)+DELTAM(JP1ML))
385.      VNIKX(L) = VM*DELTAP(L) + VMPREV
386.      26  VMPREV = VM*DELTAM(JP1ML)
387.      VNIKX(JP1) = VMPREV
388.      J = JP1
389.      I F (J .LT. JHIGH)                GO TO 20
390. C
391.      99  RETURN
392.      END
393.      SUBROUTINE INTERV(XT,LXT,X,ILEFT,MFLAG,J
399.      COMPUTES LARGEST ILEFT IN (1,LXT) SUCH THAT XT(ILEFT).LE. X
395.      DIMENSION XT(LXT)
396.      DATA ILO /1/
397.      IHI = ILO + 1
398.      I F (IHI .LT. LXT)                GO TO 20
399.      I F (X .GE. XT(LXT))              GO TO 10
400.      I F (LXT .LE. 1)                  GO TO 9 0
401.      ILO = LXT - 1
402.                                         GO TO 21
403.      20  I F (X .GE. XT(IHI))           GO TO 40
404.      21  I F (X .GE. XT(ILO))           GO TO 100
405.      C**** NOW X .LT. XT(IHI) . FIND LOWER BOUND
406.      30  ISTEP = 1
407.      31  IHI = ILO
408.      ILO = IHI - ISTEP
409.      I F (ILO .LE. 1)                  GO TO 35
410.      I F (X .GE. XT(ILO))              GO TO 50
411.      ISTEP = ISTEP*2
412.                                         GO TO 31
413.      35  ILO = 1
414.      I F (X .LT. XT(1))                GO TO 90
415.                                         GO TO 5 3
416.      C**** N O W X .GE. XT(ILO) . FIND UPPER BOUND
417.      40  ISTEP = 1
418.      41  ILO = IHI
419.      IHI = ILO + ISTEP
420.      I F (IHI .GE. LXT)                GO TO 45
421.      I F (X .LT. XT(IHI))              GO TO 50
422.      ISTEP = ISTEP*2
423.                                         GO TO 41
424.      45  I f (X .GE. XT(LXT))           GO TO 110
425.      IHI = LXT
426.      C**** NOW XT(ILO) .LE. X .LT. XT(IHI) . NAKRON THE I N T E R V A L

```

```

427.      50 MIDDLE = (ILO + IHI)/2
428.      I f (MIDDLE.EQ.ILO)          GO TO 100
429. C    NOTE. I T I S A S S U M E D THAT MIDDLE = ILO IN CASE IHI = ILO+1
433.      I F (X.LT.XT(MIDDLE))      GO TO 5 3
431.      ILO = MIDDLE
432.          GO TO 50
433.      53 IHI = MIDDLE
434.          GO TO 50
435. C**** SET OUTPUT AND RETURN
436.      9 0 MFLAG = - 1
437.      ILEFT = 1
438.          RETURN
439.      1 0 0 MFLAG = 0
440.      ILEFT = ILO
441.          RETURN
442.      110 HFLAG = 1
443.      ILEFT = LXT
444.          RETURN
445.      END

```


APPENDIX II

```

1.  PROCEDURE DEBNAT( INTEGER VALUE N1,N2,M; REAL ARRAY X(*);
2.      REAL ARRAY A(*,*); REAL ARRAY CFF(*));
3.  COMMENT DEBNAT COMPUTES THE COEFFICIENTS OF BOTH THE PIECEWISE
4.      POLYNOMIAL REPRESENTATION AND THE B-SPLINE REPRESENTATION OF A
5.      NATURAL SPLINE S(X) OF DEGREE (2*M-1), INTERPOLATING THE
6.      ORDINATES Y(I) AT POINTS X(I), I=N1 THROUGH N2.
7.      PIECEWISE POLYNOMIAL REPRESENTATION:
8.      FOR XX IN (X(N1), X(N2)), I=N1, ..., N2-1,
9.      S(XX)=A(I,0)+A(I,1)*T+...+A(I,2*M-1)*T**(2*M-1)
10.     WITH T=XX-X(I).
11.     B-SPLINE REPRESENTATION:
12.     FOR XX IN (X(N1), X(N2)),
13.     S(XX)=CFF(1)*N(1,2*M,XX)+CFF(2)*N(2,2*M,XX)+...
14.           +CFF(N2-N1+2*M-1)*N(N2-N1+2*M-1,2*M,XX)
15.     WHERE N(J,2*M,XX) IS THE (NORMALIZED) B-SPLINE OF DEGREE
16.     (2*M-1) ON THE KNOT SEQUENCE T(J), ..., T(J+2*M).
17.     INPUT:
18.     N1,N2 SUBSCRIPT OF FIRST AND LAST DATA POINT
19.     M      2*M-1 IS THE DEGREE OF THE NATURAL SPLINE,
20.           ADMISSIBLE VALUES RANGE FROM 1 TO N2-N1+1,
21.           RECOMMENDED VALUES ARE NOT GREATER THAN 7 (SAY)
22.     X(N1::N2) CONTAINS THE GIVEN ABCISSAS X(I) WHICH
23.           MUST BE STRICTLY MONOTONE INCREASING
24.     A(N1::N2,0::2*M-1) CONTAINS THE GIVEN ORDINATES AS ZERO-TH
25.           COLUMN, I.E. A(I,0) REPRESENTS Y(I),
26.     OUTPUT:
27.     A(N1::N2,0::2*M-1) THE COEFFICIENTS OF THE PIECEWISE POLYNOMIAL
28.           REPRESENTATION OF THE NATURAL SPLINE, (A(N2,0) IS
29.           UNCHANGED AND NO VALUES ARE ASSIGNED TO THE LAST
30.           ROW OF A)
31.     CFF(1::N2-N1+2*M-1) THE COEFFICIENTS OF THE B-SPLINE
32.           REPRESENTATION OF THE NATURAL SPLINE;
33.     IF (M > 0) AND (M <= N2-N1+1) THEN
34.     BEGIN
35.     PROCEDURE BSPLOR(REAL ARRAY T,A(*); INTEGER VALUE N,K;
36.           REAL ARRAY ADIF(*,*); INTEGER VALUE NDERIV);
37.     COMMENT CONSTRUCTS DIV.DIFF. TABLE FOR B-SPLINE COEFF.
38.           PREPARATORY TO DERIV.CALC.. ARRAY DIMENSIONS ARE AS
39.           FOLLOWS: T(1::N+K), A(1::N), ADIF(1::N,1::NDERIV).
40.           NDERIV SHOULD BE IN(2,K);
41.     BEGIN
42.     INTEGER KMID;
43.     REAL DIFF;
44.     FOR I:=1 UNTIL N DO ADIF(I,1):=A(I);
45.     KMID:=K;
46.     FOR ID:=2 UNTIL NDERIV DO
47.     BEGIN
48.     KMID:=KMID-1;
49.     FOR I:=ID UNTIL N DO
50.     BEGIN
51.     DIFF:=T(I+KMID)-T(I);
52.     IF DIFF=0 THEN
53.     ADIF(I, ID):=(ADIF(I, ID-1) - ADIF(I-1, ID-1))/DIFF*KMID
54.     END
55.     END
56.     END BSPLOR;
57.     PROCEDURE BSPLEV(REAL ARRAY T(*); REAL ARRAY ADIF(*,*);
58.           INTEGER VALUE N,K; REAL VALUE X;
59.           REAL ARRAY SVALUE(*); INTEGER VALUE NDERIV);
60.     COMMENT CALCULATES VALUE OF SPLINE AND ITS DERIVATIVES AT X FROM

```

```

61.          B-REPRESENTATION.  ARRAY DIMENSIONS ARE AS FOLLOWS:
62.          T(1::N+K), ADIF(1::N,1::NDERIV), SVALUE(1::NDERIV);
63.      BEGIN
64.          REAL ARRAY VNIKX(1::K);
65.          REAL ARRAY TT(1::N+1);
66.          INTEGER KML,MFLAG,I,LEFT,ID,KP1MN;
67.          FOR I DUMMY:=1 UNTIL NDERIV DO SVALUE(IDJMMY) :=0;
68.          KML:=K-1;
69.          FOR I DUMMY:=1 UNTIL N+1 DO TT(IDJMMY):=T(IDJMMY+K-1);
70.          INTERV(TT,N+1-KML,X,I,MFLAG);
71.          I:=I+KML;
72.          IF MFLAG<0 THEN GO TO S99
73.          ELSE IF MFLAG=0 THEN GO TO S20;
74.          IF X>T(I) THEN GO TO S99;
75.      S10:  IF I=K THEN GO TO S99;
76.          I:=I-1;
77.          IF X=T(I) THEN GO TO S10;
78.          COMMENT I HAS BEEN FOUND AN (K,N) SO THAT T(I)<=X<=T(I+1)
79.          (OR <=T(I+1), IF T(I)<T(I+1)=T(N+1));
80.      S20:  KP1MN:=K+1-NDERIV;
81.          BSPLVN(T,KP1MN,1,X,I,VNIKX);
82.          ID:=NDERIV;
83.      S21:  LEFT:=I-KP1MN;
84.          FOR L:=1 UNTIL KP1MN DO
85.              SVALUE(ID):=VNIKX(L)*ADIF(LEFT+L,ID) + SVALUE(ID);
86.          ID:=ID-1;
87.          IF ID=0 THEN GO TO 393;
88.          KP1MN:=KP1MN+1;
89.          BSPLVN(T,0,2,X,I,VNIKX);
90.          GO TO S21;
91.      s99 :
92.          END BSPLVN;
93.          PROCEDURE BSPLPP(REAL ARRAY T,A(*); INTEGER VALUE N,K;
94.              REAL ARRAY SCRTCH(*,*); REAL ARRAY XI(*);
95.              REAL ARRAY C(*,*); INTEGER RESULT LXI;
96.          COMMENT CONVERTS B-SPLINE REPRESENTATION TO PIECEWISE POLYNOMIAL
97.          REPRESENTATION.  ARRAY DIMENSIONS ARE AS FOLLOWS:
98.              T(1::N+K), A(1::N), SCRTCH(1::N,1::K), XI(1::LXI+1),
99.              C(1::K,1::LXI).  LXI=N-K-1 IF NO REPEATED KNOTS;
100.      BEGIN
101.          BSPLDR(T,A,N,K,SCRTCH,K);
102.          LXI:=0;
103.          XI(1):=T(K);
104.          FOR ILEFT:=K UNTIL N DO
105.              IF T(ILEFT+1)~=T(ILEFT) THEN
106.                  BEGIN
107.                      LXI:=LXI+1;
108.                      XI(LXI+1):=T(ILEFT+1);
109.                      BSPLVN(T,SCRTCH,N,K,XI(LXI),C(*,LXI),K)
110.                  END
111.          END BSPLPP;
112.          PROCEDURE BSPLVN(REAL ARRAY T(*); INTEGER VALUE JHIGH,INDEX;
113.              REAL VALUE X; INTEGER VALUE ILEFT;
114.              REAL ARRAY VNIKX(*));
115.          COMMENT CALCULATES THE VALUE OF ALL POSSIBLY NONZERO B-SPLINES AT X
116.          OF ORDER MAX(JHIGH,(JJ+1 J (INDEX-1))) UNT.  INDEX=1 OR 2.
117.          JJ, DELTAM, DELJAP ARE GLOBAL VARIABLES.
118.          BEFORE THE FIRST CALL ONE HJSJ SET JJ=1 AND ALL ELEMENTS OF
119.          DELTAM AND DELJAP = 40.  ARRAY DIMENSIONS ARE AS FOLLOWS:
120.              T(1::N+K), VNIKX(1::K), DELTAM(1::K), DELTAP(1::K);
121.      BEGIN

```

```

122.      INTEGER JP1,JP1ML;
123.      REAL VMPREV,VM;
124.      IF INDEX=1 THEN
125.      BEGIN
126.          JJ:=1;
127.          VNIKX(1):=1;
128.          IF JJ>=JHIGH THEN GO TO S99
129.      END;
130. S20:   DELTAP(JJ):=T(ILEFT+JJ)-X;
131.      DELTAM(JJ):=X-T(ILEFT-JJ+1);
132.      VMPREV:=0;
133.      JP1:=JJ+1;
134.      FOR L:=1 UNTIL J-JDU
135.      BEGIN
136.          JP1ML:=JP1-L;
137.          VM:=VNIKX(L)/(DELTAP(L)+DELTAM(JP1ML));
138.          VNIKX(L):=VM*DELTAP(L)+VMPREV;
139.          VMPREV:=VM*DELTAM(JP1ML)
140.      END;
141.      VNIKX(JP1):=VMPREV;
142.      JJ:=JP1;
143.      IF JJ<JHIGH THEN GOTOS20;
144. S99:   ENDBSPLVN;
145.      PROCEDURE BSPLVN(REAL ARRAY T(*); INTEGER VALUE K;
146.          REAL VALUE X; INTEGER VALUE ILEFT;
147.          HEAL ARRAY VNIKX(*, *); INTEGER VALUE NDERIV);
148.      COMMENT CALCULATES VALUE AND DERIVS. OF ALL B-SPLINES WHICH DO
149.      NOT VANISH AT X. ARRAY DIMENSIONS ARE AS FOLLOWS:
150.          T(1::N+K), VNIKX(1::K,1::NDERIV);
151.      BEGIN
152.          INTEGER IDERIV,IDERVM,KMD,I,J,JM1,JLW;
153.          HEALV,DIFF;
154.          REAL ARRAY NVNIKX(1::K);
155.          REAL ARRAY A(1::K,1::K);
156.          COMMENT FILL VNIKX(J,IDERIV), J=IDERIV,...,K WITH NONZERO
157.          VALUES OF B-SPLINES OF ORDER K+1-IDERIV,
158.          IDERIV=NDERIV,...,1 BY REPEATED CALLS TO BSPLVN;
159.          BSPLVN(T,K+1-NDERIV,1,X,ILEFT,NVNIKX);
160.          FOR I DUMMY:=NDERIV UNTIL K DO
161.              VNIKX(IDUMMY,NDERIV):=NVNIKX(IDUMMY-NDERIV+1);
162.          IF NDERIV<=1 THEN GOTOS99;
163.          IDERIV:=NDERIV;
164.          FOR I:=2 UNTIL NDERIV DO
165.          BEGIN
166.              IDERVM:=IDERIV-1;
167.              FOR J:=IDERIV UNTIL K DO
168.                  VNIKX(J-1,IDERVM):=VNIKX(J,IDERIV);
169.              IDERIV:=IDERVM;
170.              BSPLVN(T,0,2,X,ILEFT,NVNIKX);
171.              FOR I DUMMY:=IDERIV UNTIL K DO
172.                  VNIKX(IDUMMY,IDERIV):=NVNIKX(IDUMMY-IDERIV+1)
173.              END;
174.          FOR I:=1 UNTIL K DO
175.          BEGIN
176.              FOR J:=1 UNTIL K DO
177.                  A(I,J):=0;
178.              A(I,1):=1
179.          END;
180.          KMD:=K;
181.          FORM:=2 UNTIL NDERIV DO
182.

```

```

183.      BEGIN
184.          KMD:=KMD-1;
185.          I:=ILEF T;
185.          J:=K;
187.      S21:  JM1:=J-1;
188.          DIFF:=T(I+KMD) - T(I);
189.          IF JM1=0 THEN GO TO S26;
190.          IF DIFF=0 THEN GO TO S25;
191.          FOR L:=1 UNTIL J DO
192.              A(L,J):=I A(L,J)- A(L,J-1)/DIFF*KMD;
193.      S25:  J:=JM1;
194.          I:=I-1;
195.              GO TO S21;
196.      S26:  IF DIFF=0 THEN GO TO S30;
197.          A(1,1):=A(1,1)/DIFF*KMD;
198.      S30:  FOR I:=1 UNTIL K DO
199.          BEGIN
200.              V:=0;
201.              JLOW:=IF I>=M THEN I ELSE M ;
202.              FOR J:=JLOW UNTIL K DO
203.                  V:=A(I,J)*VNIKX(J,M) + V;
204.                  VNIKX(I,M):=V
205.              END;
206.          END;
207.      s99:  END BSPLVO;
208.          PROCEDURE INTERV(REAL ARRAY XT(*);INTEGER VALUE LXT;REAL VALUE X;
209.              INTEGER RESULT ILEF T, MFLAG);
210.          COMMENT COMPUTES LARGEST ILEFT IN(1,LXT) SUCH THAT XT(ILEFT)<=X.
211.              XT IS OF SIZE XT(1::LXT). ILO IS A GLOBAL VARIABLE.
212.              ILO MUST BE SET EQUAL TO 01 BEFORE THE FIRST CALL TO INTERV;
213.
214.      BEGIN
215.          INTEGER IHI,ISTEP,MIDDLE;
216.          IHI:=ILO+1;
217.          IF IHI<LXT THEN GO TO S20;
218.          IF X>=XT(LXT) THEN GO TO S110;
219.          IF LXT<=1 THEN GO TO S90;
220.          ILO:=LXT-1;
221.              GO TO S21;
222.      S20:  IF X>=XT(IHI) THEN GO TO S40;
223.      S21:  IF X>=XT(ILO) THEN GO TO S100;
224.          COMMENT NOW X<XT(IHI). FIND LOWER BOUND;
225.      S30:  ISTEP:=1;
226.      s31:  IHI:=ILO;
227.          ILO:=IHI-ISTEP;
228.          IF ILO<=1 THEN GO TO S35;
229.          IF X>=XT(ILO) THEN GO TO S50;
230.          ISTEP:=ISTEP*2;
231.              GO TO S31;
232.      s35:  ILO:=1;
233.          IF X<XT(1) THEN GO TO S90;
234.              GO TO S50;
235.          COMMENT NOW X>=XT(ILO). FIND UPPER BOUND;
236.      S40:  ISTEP:=1;
237.      S41:  ILO:=IHI;
238.          IHI:=ILO+ISTEP;
239.          IF IHI>=LXT THEN GO TO S45;
240.          IF X<XT(IHI) THEN GO TO S50;
241.          ISTEP:=ISTEP*2;
242.              GO TO S41;
243.      s45:  IF X>=XT(LXT) THEN GO TO S110;

```

```

244.      IHI:=LXT;
245.      COMMENT NOW XT(ILO)<=X<XT(IHI).  NARROW THE INTERVAL;
246. S50:  MIDDLE:=(ILO+IHI) DIV 2;
247.      IF MIDDLE=ILO THEN GO TO S100;
248.      COMMENT IT IS ASSUMED THAT MIDDLE=ILO IN CASE IHI=ILO+1;
249.      IF X<XT(MIDDLE) THEN GO TO S53;
250.      ILO:=MIDDLE;
251.                               GO TO S50;
252. S53:  IHI:=MIDDLE;
253.                               GO TO S50;
254.      CCMMEN T S E T C U T P U T A N D E X I T;
255. S90:  MFLAG:=-1;
255.      ILEFT:=1;
257.                               GO TO SFIN;
258. S100: MFLAG:=0;
259.      ILEFT:=ILO;
263.                               GO TO SFIN;
261. S110: MFLAG:=1;
262.      ILEFT:=LXT;
263. SFIN:
264.      END INTERV;
265.      PROCEDURE BANDET (REAL ARRAY M(*,*); INTEGER ARRAY INT(*);
266.                          REAL AR941 A(*,*); INTEGER VALUE N,M1,M2);
267.      COMMENT BANOET AND ITS COMPANION PROCEDURE BANSOL SOLVE THE SYSTEM
268.      O F E Q U A T I O N S  $A \cdot X = B$  WHERE A IS A NONSYMMETRIC BAND MATRIX.
269.      (THEY WILL WORK WITH SYMMETRIC BAND MATRICES BUT TAKE NO
273.      ADVANTAGE OF THEIR STRUCTURE.)
271.      T H E B A N D M A T R I X 4 O F O R D E R N W I T H M 1 S U B - D I A G O N A L E L E M E N T S
272.      A N O M 2 S U P E R - D I A G O N A L E L E M E N T S I N A T Y P I C A L R O W I S S T O R E D A S
273.      A N N B Y (M1+M2+1) ARRAY, A(1::N,1::M1+M2+1), W I T H T H E
274.      S U B - D I A G O N A L E L E M E N T S I N A(*,J), J=1,...,M1, T H E D I A G O N A L
275.      E L E M E N T S I N A(*,M1+1), A N D T H E S U P E R - D I A G O N A L E L E M E N T S I N
275.      A(*,J), J=M1+2,...,M1+M2+1. T H E M A T R I X A I S F A C T O R I Z E D B Y
277.      B A N D E T I N T O T H E P R O D U C T O F A L O W E R - T R I A N G U L A R M A T R I X A N O A N
278.      U P P E R - T R I A N G U L A R M A T R I X U S I N G P A R T I A L P I V O T I N G. T H E L O W E R
279.      T R I A N G L E I S S T O R E D A S A N N B Y M 1 A R R A Y M(1::N,1::M1) A N O T H E
283.      U P P E R T R I A N G L E I S O V E R W R I T T E N O N A. D E T A I L S O F T H E
281.      I N T E R C H A N G E S A R E S T O R E D A N T H E A R R A Y I N T(1::N);
2 8 2 .      BEGIN
283.          INTEGER I,L,M3;
284.          REAL X;
285.          M3:=M1+M2+1;
286.          L:=M1;
287.          FOR I:=1 UNTIL M 1 D O
289.              BEGIN
289.                  FOR J:=M1+2-I U N T I L M 3 D O
290.                      A(I,J-L):=A(I,J);
291.                  L:=L-1;
292.                  FOR J:=M3-L U N T I L M 3 D O
293.                      A(I,J):=C
294.              END I ;
295.          L:=M1;
296.          FOR K:=1 UNTIL N 0 0
297.              BEGIN
298.                  X:=A(K,1);
299.                  I:= ;
303.                  IF L<N T H E N L:=L+1;
301.                  FOR J:=K+1 U N T I L L 3 3
302.                      I F A B S ( A ( J , 1 ) ) > A B S ( X ) T H E N
303.                          BEGIN
304.                              X:=A(J,1);

```



```

365. REAL ARRAY TRL (1::N2-N1+2*M-3,1::M-1);
367. REAL ARRAY VNIKX(1::2*M,1::2*M-1);
368. REAL ARRAY C(1::2*M,1::N2-N1+1);
369. INTEGER ARRAY INT(1::N2-N1+2*M-3);
373. TN2:=N2-N1+1;
371. TM2:=2*M;
372. TN4:=TN2+TM2-4;
373. TMM:=TM2-1;
374. FOR I:=N1 UNTIL N2 DO
375. BEGIN
376. TX(I-N1+1):=X(I);
377. TY(I-N1+1):=A(I,0)
378. END I;
379. JJ:=ILO:=1;
380. FOR I:=1 UNTIL TM2 DO DELTAM(I):=DELTAP(I):=40;
381. FOR I:=1 UNTIL TMM DO T(I):=TX(I);
382. FOR I:=1 UNTIL TN2-1 DO T(I+TMM):=TX(I);
383. TN3:=TN2-1+TMM;
384. FOR I:=1 UNTIL TM2 DO T(I+TN3):=TX(TN2);
385. COMMENT GET COEFFICIENTS OF FIRST M-1 ROWS;
386. BSPLVD(T, TM2, TX(1), TM2, VNIKX, TMM);
387. A1:=TY(1)/VNIKX(1,1);
388. FOR I:=1 UNTIL M-1 DO
389. BEGIN
390. FOR J:=1 UNTIL TMM DO Q(I,J):=0;
391. MPI:=M+I;
392. LL:=M-I;
393. FOR L:=2 UNTIL MPI DO
394. BEGIN
395. LL:=LL+1;
396. Q(I,LL):=VNIKX(L,MPI)
397. END L;
398. TA(I):=-A1*VNIKX(1,MPI)
399. END I;
400. COMMENT GET COEFFICIENTS OF NEXT TN2 ROWS;
401. MM2:=M-2;
402. FOR I:=2 UNTIL TN2-1 DO
403. BEGIN
404. BSPLVN(T, TM2, 1, TX(I), I+TMM, VNIKX(*,1));
405. IM2:=I+MM2;
406. FOR L:=1 UNTIL TMM DO Q(IM2,L):=VNIKX(L,1);
407. TA(IM2):=TY(I)
408. END I;
409. COMMENT GET COEFFICIENTS OF LAST M-1 ROWS;
410. BSPLVD(T, TM2, TX(TN2), TN3, VNIKX, TMM);
411. ANP:=TY(TN2)/VNIKX(TM2,1);
412. FOR I:=1 UNTIL M-1 DO
413. BEGIN
414. II:=TN2+TM2-3-I;
415. FOR J:=1 UNTIL TMM DO Q(II,J):=0;
416. MPI:=M+I;
417. LL:=M-I;
418. FOR L:=1 UNTIL MPI-1 DO
419. BEGIN
420. LL:=LL+1;
421. Q(II,LL):=VNIKX(LL,MPI)
422. END L;
423. TA(II):=-ANP*VNIKX(TM2,MPI)
424. END I;
425. BANDET(TRL, INT, Q, TN4, M-1, M-1);
426. BANSOL(TRL, INT, TA, Q, TN4, M-1, M-1);

```

