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## Minimal Norm

### Constrained Interpolation

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## A Dissertation Submitted to the Faculty of Old Dominion University in Partial Fulfillment of the Requirements for the Degree of

Doctor of Philosophy

Computational and Applied Mathematics

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Approved hv:

Philip W. Smith (Director)

#### ABSTRACT

#### MINIMAL NORM CONSTRAINED INTERPOLATION

Larry Dean Irvine Old Dominion University, 1985 Director: Dr. Philip W. Smith

In computatonal fluid dynamics and in CAD/CAM a physical boundary, usually known only discreetly (say, from a set of measurements), must often be approximated. An acceptable approximation must, of course, preserve the salient features of the data (convexity, concavity, etc.) In this dissertation we compute a smooth interpolant which is locally convex where the data are locally convex and is locally concave where the data are locally concave.

Such an interpolant is found by posing and solving a minimization problem. The solution is a piecewise cubic polynomial. We actually solve this problem indirectly by using the Peano kernel theorem to recast this problem into an equivalent minimization problem having the second derivative of the interpolant as the solution.

We are then led to solve a nonlinear system of equations. We show that with Newton's method we have an exceptionally attractive and efficient method for solving this nonlinear system of equations.

We display examples of such interpolants as well as convergence results obtained by using Newton's method. We list a FORTRAN program to compute these shape-preserving interpolants.

Next we consider the problem of computing the interpolant of minimal norm from a convex cone in a normed dual space. This is an extension of de Boor's work on minimal norm unconstrained interpolation.

Dedication

To Dr. Philip Smith for his help and guidance.

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#### 1. The Natural Spline Interpolant

We consider the problem of computing an interpolant to given data. Throughout our discussion we shall denote the data

$$(t_{i}, y_{j})$$
  $i = 1, 2, ..., n$ 

where  $a = t_1 < t_2 < \ldots < t_n = b$  and in this chapter we place no restrictions on the numbers  $y_i$ . There are, of course, many such interpolants which we can form. For example, we can calculate the unique polynomial p of order n (degree n-1 or less) which interpolates the data. However, as pointed out in [deB(1), chapter 2], for large n (and especially for equally spaced points  $t_i$ ) the polynomial interpolant is notorious for large changes in its first derivative near the endpoints. Figure (1.1) displays the polynomial interpolant to the function

$$f(t) = \frac{1 - \sin(7 \pi t)}{2}$$

at the points  $t_i = (i-1)/10$  for i = 1, 2, ..., 11. Since  $0 \le y_i \le 1$  for each i, we expect a good interpolant to remain reasonably close to these bounds. However, because of its behavior near the endpoints, the polynomial interpolant fails to model the data well. This behavior is typical of high-order polynomial interpolants.

In order to decrease the unnaturally large changes in the first derivative characteristic of the polynomial interpolant, we wish to calculate the interpolant which "bends" the least over all suitable interpolants. The norm of the second derivative of an interpolant will furnish a measure of the bending of the interpolant so we pose a minimization problem on  $L_2^{(2)}[a,b]$ , the Sobolev space of functions with



Figure (1.1): The Polynomial Interpolant.

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second derivatives in the normed linear space  $L_2[a,b]$ . Let A denote the set of all interpolants in the Sobolev space. We consider the minimization problem

Find  $f_* \varepsilon A$  such that  $\|f_*^{(2)}\|_2 \leq \|f^{(2)}\|_2$  for all  $f \varepsilon A$ . (1.1) We shall see that the solution to (1.1) is piecewise cubic with two

continuous derivatives; that is

$$f_{*}(t) = p_{i}(t)$$
 if  $t_{i} \leq t \leq t_{i+1}$ 

for i = 1,2,...,n-1 where  $p_i$  is a cubic polynomial and  $f_*$  is in  $C^2[a,b]$ . We follow the pattern in [deB(1), chapter 5], taking advantage of the fact that  $L_2[a,b]$  is not only a normed linear space, but also a Hilbert space with an inner product defined by

$$(f,g) = \int_{a}^{b} f(t)g(t)dt$$

for any two elements f and g in  $L_2[a,b]$ .

Assume f is an element of A. (The set A is nonempty since it contains the polynomial interpolant.) We shall use the Peano kernel theorem to obtain a set of equations for  $f^{(2)}$ . By the Fundamental Theorem of Calculus we have

$$f(t) = f(a) + \int_{a}^{t} f^{(1)}(s) ds$$
 (1.2)

We integrate  $\int_{a}^{t} f^{(1)}(s) ds$  by parts noting that  $\int u dv = uv - \int v du$ .

Let

$$u(s) = f^{(1)}(s)$$
 and  $dv(s) = ds$ 

so that

$$du(s) = f^{(2)}(s)ds$$
 and  $v(s) = -(t-s)$ 

where t is a constant. Hence

$$\int_{a}^{t} f^{(1)}(s) ds = (t-a) f^{(1)}(a) + \int_{a}^{t} f^{(2)}(s) ds$$

and so (1.2) becomes

$$f(t) = q_{1}(t) + \int_{a}^{t} (t-s)f^{(2)}(s)ds \qquad (1.3)$$

where  $q_1(t) = f(a) + f^{(1)}(a)(t-a)$ . (This is actually a Taylor's series with integral remainder.)

To acquire constant limit of integration we can write (1.3) as

$$f(t) = q_1(t) + \int_a^b (t-s)_+ f^{(2)(s)ds}$$
(1.4)

where  $(h)_{+}$ , the positive part of the function h, is defined by

$$(h)_{+}(t) = \begin{cases} h(t) & \text{if } h(t) \ge 0\\ 0 & \text{if } h(t) \le 0. \end{cases}$$

Now we consider the divided difference operator. Given a function g and a set of points  $\{\tau_i, \tau_{i+1}, \dots, \tau_{i+m}\}$ , the m-th divided difference of g - denoted by  $[\tau_i, \tau_{i+1}, \dots, \tau_{i+m}]g(\cdot)$  - is the leading coefficient of the polynomial of order m+1 which interpolates g at  $\tau_i, \tau_{i+1}, \dots, \tau_{i+m}$ (and hence is a function of  $\tau_i, \tau_{i+1}, \dots, \tau_{i+m}$ ). The recursive relations

$$[\tau_{p}]g(\bullet) = g(\tau_{p})$$

$$[\tau_{i},\tau_{i+1},\ldots,\tau_{i+m}]g(\bullet) = \frac{[\tau_{i+1},\ldots,\tau_{i+m}]g(\bullet) - [\tau_{i},\ldots,\tau_{i+m-1}]g(\bullet)}{\tau_{i+m} - \tau_{i}}(1.5)$$

hold if  $\tau_{i+m} \neq \tau_i$  (which we assume for our data). Presently we are interested in the case m=2. Equation (1.5) becomes (with  $\tau_i = t_i$ )

$$(t_{i+2} - t_i)[t_i, t_{i+1}, t_{i+2}]g(\bullet) = \frac{g(t_{i+2}) - g(t_{i+1})}{t_{i+2} - t_{i+1}} - \frac{g(t_{i+1}) - g(t_i)}{t_{i+1} - t_i}$$
(1.6)

which is computable for i=1,2,...,n-2.

Notice that  $[\tau_i, \tau_{i+1}, \dots, \tau_{i+m}]p(\bullet) = 0$  if p is a polynomial of order m or less (degree m-l or less). (From equation (1.6) we see that  $(t_{i+2} - t_i)[t_i, t_{i+1}, t_{i+2}]g(\bullet)$  measures a difference in slopes; the difference in slopes being zero if g is linear.)

Now we apply the (scaled) second-divided difference operator  $(t_{i+2} - t_i)[t_i, t_{i+1}, t_{i+2}]$  to (1.4) and interchange the order of the integral and divided difference operators to obtain

$$d_{i,2} = \int_{a}^{b} g(s)N_{i}(s)ds \quad i=1,2,\ldots,n-2$$
 (1.7)

where

$$d_{i,2} = (t_{i+2} - t_i)[t_i, t_{i+1}, t_{i+2}]f(\cdot)$$

$$= \frac{y_{i+2} - y_{i+1}}{t_{i+2} - t_{i+1}} - \frac{y_{i+1} - y_i}{t_{i+1} - t_i} , \qquad (1.8)$$

$$N_{i,2}(\cdot) = (t_{i,2} - t_i)[t_i, t_{i+1}, t_{i+2}](\cdot -s)_{+}$$

$$=\frac{(t_{i+2} - s)_{+} - (t_{i+1} - s)_{+}}{t_{i+2} - t_{i+1}} - \frac{(t_{i+1} - s)_{+} - (t_{i} - s)_{+}}{t_{i+1} - t_{i}}$$
(1.9)

and  $g = f^{(2)}$ . We call  $N_{i,2}$  the (normalized) linear B-spline (or B-spline of order 2) with knots  $t_i$ ,  $t_{i+1}$  and  $t_{i+2}$ . The graph of  $N_{i,2}$ is displayed in figure (1.2).



Figure (1.2): The Normalized Linear B-spline.

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We have shown that if f is an interpolant in the Sobolev space (f  $\epsilon$  A), then g = f<sup>(2)</sup> satisfies (1.7). Let the set B consist of all functions which are in L<sub>2</sub>[a,b] and which satisfy (1.7).

Now consider the problem

Find  $g_* \in B$  such that  $||g_*||_2 \leq ||g||_2$  for all  $g \in B$  (1.10) A unique solution exists since (1.10) is a minimal norm problem over a nonempty closed convex set in a Hilbert space. Furthermore, the solutions of problems (1.1) and (1.10) are related via  $g_* = f_*^{(2)}$ . Hence, to compute  $f_*$  we can first calculate  $g_*$  and then integrate  $g_*$ twice. Since much of our emphasis will be on  $g_*$ , rather than  $f_*$ , we shall call  $g_*$  the interpolant of minimal norm.

For brevity we denote the index m = n-2, the B-spline  $N_i = N_{i,2}$ , and the divided difference  $d_i = d_{i,2}$ . We also define the vector-valued function T:L<sub>2</sub>[a,b]  $\rightarrow R^m$  by

$$(Tx)_{i} = \int_{a}^{b} x(t)N_{i}(t)dt \quad i=1,2,\ldots,m.$$

To solve problem (1.10) we shall show that  $g_{x}$ , the interpolant of minimal norm, is the intersection of two specific sets--one an orthogonal complement of a subspace and the other a translate of a subspace --in  $L_{2}[a,b]$  via a variation of the Projection Theorem. If W is a closed subspace of a Hilbert space H and if x is an arbitrary element of H, then the Projection Theorem states that there exists a unique element w<sub>o</sub> in W satisfying

$$\|\mathbf{x} - \mathbf{w}_{0}\| \leq \|\mathbf{x} - \mathbf{w}\| \quad \text{for all } \mathbf{w} \in \mathbb{W}$$
 (1.11)

and characterized by

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$$(x - w_0, w) = 0$$
 for all  $w \in W$ .

Hence  $x - w_0$  is in W<sup>1</sup>, the orthogonal complement of W. The proof of the Projection Theorem can be found in any book dealing with Hilbert spaces (for example, [L, page 517]). The next proposition will serve as the actual form of the Projection theorem which we shall use.

<u>Proposition</u> ([L, page 64]): Let W be a closed subspace in a Hilbert <u>space</u> H. For a fixed element x in H define V: = x + W. Then there <u>exists a unique element</u> x<sub>0</sub> in V of minimal norm. Furthermore, x<sub>0</sub> is <u>in</u> W<sup>1</sup>.

(The translate V is called an affine set or linear variety.) Notice that  $x_0$  is the intersection of the orthogonal complement of W and the translate V of W. In fact, (1.11) reveals that  $x_0 = x - w_0$ .

Define

$$W: = \{z \in L_2[a,b] : Tz = \theta\}$$

which is a closed subspace in  $L_2[a,b]$ . Let  $g \in L_2[a,b]$  be any element such that  $Tg = \underline{d}$ . (Equivalently, let g be any element of B.) Then B = g + W and B corresponds to the linear variety in the proposition. Hence  $g_*$  is the unique element in  $W^{\perp}$  satisfying  $Tg_* = \underline{d}$ .

We consider the contents of W<sup> $\perp$ </sup>. Any element which is orthogonal to each N<sub>i</sub> is also orthogonal to any linear combination of the Bsplines. Hence S: = span(N<sub>1</sub>, N<sub>2</sub>,..., N<sub>m</sub>) is a subset of W<sup> $\perp$ </sup>. We now show that W<sup> $\perp$ </sup> is a subset of S (and hence S = W<sup> $\perp$ </sup>) by contradiction. Assume that there exists an element y which is in W<sup> $\perp$ </sup> but not in S. Since S is a closed subspace there exists (by the Projection Theorem)

an element  $s_0$  in S such that

with  $y - s_0$  in the orthogonal complement of S. This implies  $T(y - s_0) = \theta$  or  $(y - s_0) \in W$ . However  $y - s_0$  is also in  $W^{\perp}$  since both y and  $s_0$  are in  $W^{\perp}$ . Therefore  $(y - s_0) = \theta$  and  $S = W^{\perp}$ .

In summary,  $\mathbf{g}_{\mathbf{x}}$  is characterized by

$$g_* = \sum_{i=1}^{m} \alpha_i N_i$$

(since  $g_*$  is in the span of the B-splines) where the coefficients  $\alpha_1, \alpha_2, \ldots, \alpha_m$  are chosen to satisfy

$$\binom{m}{\sum_{j=1}^{m} \alpha_{j} N_{j}, N_{i}} = d_{i} \quad i=1,2,...,m$$
 (1.12)

(since  $Tg_* = \underline{d}$ ). Equation (1.13), a system of m linear equations in m unknowns, can be written in matrix notation as

$$A\underline{\alpha} = \underline{d} \tag{1.13}$$

where the symmetric matrix A has entries  $A_{ij} = (N_i, N_j)$ .

Because the B-splines are linearly independent, the matrix A, a Grahm matrix, is nonsingular and hence a unique solution exists for any given <u>d</u>. Furthermore, since N<sub>i</sub> has support  $[t_i, t_{i+2}]$ , the matrix A is tridiagonal. For any  $\underline{x} \in \mathbb{R}^m$  we have

$$\underline{\mathbf{x}}^{\mathrm{T}}\underline{\mathbf{A}}\underline{\mathbf{x}} = \sum_{i=1}^{m} \mathbf{x}_{i} (\underline{\mathbf{A}}\underline{\mathbf{x}})_{i}$$
$$= \sum_{i=1}^{m} \mathbf{x}_{i} (\underline{\mathbf{N}}_{i}, \sum_{j=1}^{m} \mathbf{x}_{j} \underline{\mathbf{N}}_{j})$$
$$= (\sum_{i=1}^{m} \mathbf{x}_{i} \underline{\mathbf{N}}_{i}, \sum_{j=1}^{m} \mathbf{x}_{j} \underline{\mathbf{N}}_{j})$$
$$= ||\sum_{i=1}^{m} \mathbf{x}_{i} \underline{\mathbf{N}}_{i}||_{2}^{2}$$

with equality holding if and only if  $\underline{x} = \theta$ . The matrix A is hence positive definite and (1.13) can be solved by Gauss elimination without pivoting, or, better still, by Cholesky decomposition.

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We note also that

$$|| g_* || = \underline{\alpha}^T A \underline{\alpha} = \underline{\alpha}^T \underline{d}.$$

The entry  $A_{ij}$ , the integral of the product of two piecewise linear polynomials, can be computed exactly by Simpson's rule applied on each subinterval  $[t_k, t_{k+1}]$ . Denoting  $\Delta t_k := t_{k+1} - t_k$  and  $z_k$  the midpoint of the interval  $[t_k, t_{k+1}]$  we have for i=1,2,...,m

$$A_{ii} = \int_{t_{i}}^{t_{i+1}} N_{i}(t)^{2} dt + \int_{t_{i+1}}^{t_{i+2}} N_{i}(t)^{2} dt$$
  
=  $(\Delta t_{i+1}/6) [N_{i}(t_{i})^{2} + 4N_{i}(z_{i})^{2} + N_{i}(t_{i+1})^{2}]$   
+  $(\Delta t_{i+2}/6) [N_{i}(t_{i+1})^{2} + 4N_{i}(z_{i+1})^{2} + N_{i}(t_{i+2})^{2}]$   
=  $(t_{i+2} - t_{i})/3.$ 

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We also compute for i=1,2,...,m-1

$$A_{i,i+1} = A_{i+1,i}$$
$$= \int_{t_{i+1}}^{t_{i+2}} N_i N_{i+1}(t) dt$$

$$= (t_{i+2} - t_{i+1})/6.$$

The solution  $g_*$ , being a linear combination of linear B-splines, is piecewise linear (and continuous) with knots  $t_i$ . After integrating  $g_*$  twice and applying the interpolation conditions, we obtain  $f_*$  which is piecewise cubic (with knots  $t_i$ ) with two continuous derivatives.

Define  $\underline{\beta} \in R^n$  via

$$\beta_{i} = \begin{cases} 0 & i=1 \\ \alpha_{i-1} & i=2,3,\ldots,n-2 \\ 0 & i=n \end{cases}$$

and  $\Delta\beta = \beta_{i+1} - \beta_i$ . On  $[t_i, t_{i+1}] f_*$  is defined by a unique cubic polynomial  $p_*$  and hence  $f_*$  can be determined by specifying the numbers  $p_{*i}^{(j)}(t_i)$  for i=1,2,...,n-1 and j=0,1,2,3. Then

$$f_{*}(t) = \frac{p_{*i}(2)(t_{i})}{0!} + \frac{p_{*i}(t_{i})}{1!} (t-t_{i})$$

$$+ \frac{p_{*i}^{(2)}(t_{i})(t-t_{i})^{2}}{2!} + \frac{p_{*i}^{(3)}(t_{i})(t-t_{i})^{3}}{3!}$$
(1.14)

for  $t \in [t_i, t_{i+1}]$ . Of course, (1.14) can be more efficiently evaluated by using nested multiplication.

The polynomial  $\textbf{p}_{\textbf{\texttt{x}}_1}$  solves the differential equation

$$p_{*i}^{(2)}(t) = \beta_{i} + (\Delta \beta_{i} / \Delta t_{i})(t - t_{i})$$
(1.15)

on the interval  $[t_i, t_{i+1}]$  with boundary conditions  $p_{*i}(t_i) = y_i$  and  $p_{*i}(t_{i+1}) = y_{i+1}$ . Therefore

$$p_{*i}(t) = \frac{\beta_{i}}{2} (t - t_{i})^{2} + \frac{\Delta \beta_{i}}{6\Delta t_{i}} (t - t_{i})^{3} + c_{i}(t - t_{i}) + e_{i}$$
(1.16)

where the constants  $c_i$  and  $e_i$  are evaluated as  $e_i = y_i$  and

$$c_{i} = \frac{\Delta y_{i}}{\Delta t_{i}} - \left(\frac{\beta_{i+1}}{2} + \frac{\Delta \beta_{i}}{6}\right) \Delta t_{i}$$
(1.17)

with  $\Delta y_i = y_{i+1} - y_i$ . From (1.17) we obtain

$$p_{*i}^{(0)}(t_{i}) = y_{i}$$

$$p_{*i}^{(1)}(t_{i}) = c_{i}$$

$$p_{*i}^{(2)}(t_{i}) = \beta_{i}$$

$$p_{*i}^{(3)}(t_{i}) = \Delta\beta_{i}/\Delta t_{i}$$
(1.18)

where  $c_i$  is given by (1.17). A complete FORTRAN program for computing the natural cubic spline interpolant is given in Appendix A.

Figure (1.3) displays the natural cubic spline interpolant that is in contrast to the polynomial interpolant of figure (1.1).

We complete this chapter by posing (and solving) a generalization of problem (1.1). For k fixed satisfying  $2 \le k \le n$ , let A(k) be the be the set of interpolants (to the data) which are in  $L_2^{(k)}[a,b]$ . We



Figure (1.3): The Natural Cubic Spline Interpolant.

Find 
$$f_* \in A(k)$$
 such that  $\|f_*^{(k)}\|_2 \le \|f^{(k)}\|_2$  for all  $f \in A(k)$   
(1.19)

Let f be an element of A(k). Since (1.3) is valid for f, we can integrate by parts again (assuming k > 2) to obtain

$$f(t) = q_{2}(t) + \int_{a}^{t} \frac{(t-s)^{2}}{2!} f^{(3)}(s) ds \qquad (1.20)$$

where

$$q_2(t) = f(a) + f^{(1)}(a)(t-a) + \frac{f^{(2)}(a)}{2!} (t-a)^2.$$

In general, after integrating by parts k-l times we obtain

$$f(t) = q_{k-1}(t) + \int_{a}^{b} \frac{(t-s)^{k-1}}{(k-1)!} f^{(k)}(s) ds \qquad (1.21)$$

or

$$f(t) = q_{k-1}(t) + \int_{a}^{b} \frac{(t-s)_{+}^{k-1}}{(k-1)!} f^{(k)}(s) ds. \qquad (1.22)$$

$$d_{i,k} = \int_{a}^{b} g(s)N_{i,k}(s)ds$$
 i=1,2,...,n-1 (1.23)

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where

$$d_{i,k} = (k-1)!(t_{i+k}-t_i)[t_{i,\dots,t_{i+k}}]f(\cdot) , \qquad (1.24)$$

$$N_{i,k}(s) = (t_{i+k} - t_i)[t_{i,\dots,t_{i+k}}](\cdot - s)_{+}^{k-1}$$
(1.25)

(the normalized B-spline of order k), and  $g = f^{(2)}$ .

Let B(k) denote the set of elements (in  $L_2[a,b]$ ) wich satisfy (1.23). Then the solution  $f_*$  to (1.20) is related to the solution to the problem

Find  $g_* \in B(k)$  such that  $||g_*^{(k)}||_2 \leq ||g^{(k)}||_2$  for all  $g \in B(k)$  (1.26) via  $g_* = f_*^{(k)}$ . Furthermore, for some  $\underline{\alpha} \in \mathbb{R}^{n-k}$  we have

$$g_* = \sum_{j=1}^{n-k} \alpha_j^{N} j, k$$

The coefficients  $\alpha_1, \alpha_2, \dots, \alpha_{n-k}$  are chosen to solve the linear system of n-k equations in n-k unknowns represented by the matrix equation A  $\underline{\alpha} = \underline{d}$  where A is symmetric and positive definite with entries

$$A_{ij} = (N_{i,k}, N_{j,k}).$$

Since  $g_*$  is a linear combination of piecewise polynomials of order k,  $f_*$  will be a piecewise polynomial of order 2k. We call  $f_*$  the natural spline interpolant of order 2k.

## 2. <u>A Minimal Norm Interpolation Problem</u> <u>in the L [a,b] Spaces</u>

For p such that 1 we define the set

$$G(p): = \left\{ g \in L_p[a,b]: \int_a^b g(t)\phi_i(t)dt = \int_a^b g_o(t)\phi_i(t)dt \right\}$$
for i=1,2,...,n 
$$\left\{ for = 1,2,\ldots,n \right\}$$
(2.1)

where  $\{\phi_i\}_{i=1}^n$  is a set of elements in  $L_q[a,b]$ , q is conjugate to p (p+q = pq if  $p^{\neq \infty}$  and q=l if  $p = \infty$ ), and  $g_0$  is a fixed element of  $L_p[a,b]$ . Consider the problem

Find  $g_* \in G(p)$  such that  $||g_*||_p \le ||g||_p$  for all  $g \in G(p)$ . (2.2)

In chapter 1 we solved (2.2) for the special case p=2; finding from a linear variety in a Hilbert space the element of minimal norm. The Projection Theorem came in handy to characterize  $g_{x}$  as well as to guarantee uniqueness. However, for  $p \neq 2 L_{p}[a,b]$  does not have the orthogonality properties of a Hilbert space and hence, we cannot use the Projection Theorem to solve (2.2). Instead we solve (2.2) in this chapter by utilizing the Hahn-Banach theorem to characterize  $g_{x}$ . Uniqueness follows in the case 1 by the strict convexity of thenorm. This chapter, modeled after [deB(2)], motivates the use of the

Let  $\lambda$  be the linear functional defined on the subspace

Hahn-Banach theorem in chapter 5.

S: = span(
$$\phi_1, \ldots, \phi_n$$
)

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via

$$\lambda(\sum_{i=1}^{n}\alpha_{i}\phi_{i}) = \int_{a}^{b} \prod_{i=1}^{n}\alpha_{i}\phi_{i}(t)g_{0}(t)dt.$$
(2.3)

Any element of G(p) (including  $g_0$ ) will serve as an extension of  $\lambda$  to a bounded linear functional defined on all of  $L_{g}[a,b]$ . Hence,

$$\|\lambda\|_{s} \leq \|g\|_{p}$$
 for all gcG(p). (2.4)

Conversely, any extension of  $\lambda$  to a bounded linear functional defined on all of L<sub>q</sub>[a,b], being identical to  $\lambda$  on S, is represented by an element of G(p).

The Hahn-Banach theorem guarantees the existence of an element  $\hat{g} \, \epsilon \, G(p)$  such that

$$\int_{a}^{b} f(t)\hat{g}(t)dt \leq ||\lambda||_{s} \cdot ||f||_{q} \text{ for all } f \in L_{q}[a,b].$$

This implies that  $\|\hat{g}\| \leq \|\lambda\|_{s}$  which, taken along with (2.4), gives us  $\|\hat{g}\| = \|\lambda\|_{s}$  and, therefore, a solution to (2.2). Now we characterize  $\hat{g}$ .

Let  $\sum_{i=1}^{n} \alpha_{i}^{*} \phi_{i}$  be an element such that i=1

$$\left\| \sum_{i=1}^{n} \alpha_{i} \phi_{i} \right\|_{q} = 1 \quad \text{and} \quad \lambda(\sum_{i=1}^{n} \alpha_{i} \phi_{i}) = \|\lambda\|_{s}.$$

(This element is unique if 1 since the norm is strictly convex.) Then

$$\begin{split} \|\hat{g}\|_{p} &= \|\lambda\|_{s} \\ &= \lambda (\sum_{i=1}^{n} \alpha_{i} \phi_{i}) \\ &= \int_{a}^{b} (\sum_{i=1}^{n} \alpha_{i} \phi_{i}) (t) \hat{g}(t) dt \\ &\leq \|\sum_{n=i}^{n} \alpha_{i} \phi_{i}\| \cdot \|\hat{g}\|_{p} \\ &= \|\hat{g}\|_{p} . \end{split}$$

Therefore, equality holds throughout and we have

$$\int_{a}^{b} (\sum_{i=1}^{n} \alpha_{i} \phi_{i})(t) \hat{g}(t) dt = \left\| \sum_{i=1}^{n} \alpha_{i} \phi_{i} \right\|_{q} \cdot \left\| \hat{g} \right\|_{p}.$$

Since  $\hat{g}$  and  $\sum_{i=1}^{n} \alpha_{i} \phi_{i}$  are aligned, we must have

$$\hat{g}(t) = \|\lambda\|_{s} \cdot \|\sum_{i=1}^{n} \alpha_{i} \phi_{i}\|^{q-1} \operatorname{signum} (\sum_{i=1}^{n} \alpha_{i} \phi_{i})(t).$$

We close this chapter by stating the interpolation problem that goes along with solving (2.2). Let p be a number such that 1 , $let k be an integer such that <math>k \ge 2$ , and let  $f_0 \in L_p^{(k)}[a,b]$ . Define the sets

F: = {
$$f \in L_p^{(k)}[a,b]$$
:  $f(t_i) = f_o(t_i)$  i=1,2,...,n}

G: = {g 
$$\in L_p[a,b]$$
:  $\int_a^b g(t)N_{i,k}(t)dt = d_{i,k}$  i=1,2,...,n-k}

Then the problems

Find 
$$f_* \in F$$
 such that  $\|f_*^{(k)}\|_p \leq \|f^{(k)}\|_p$  for all  $f \in F$ 

and

Find 
$$f_* \in G$$
 such that  $\|g_*\|_p \leq \|g\|_p$  for all  $g \in G$ 

are equivalent and

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$$g_{*}(t) = f_{*}^{(k)}(t) = \begin{vmatrix} n-k \\ \Sigma \beta i N_{i,k} \end{vmatrix} \begin{vmatrix} q-1 & n-k \\ signum & (\Sigma \beta i N_{i,k})(t). \\ i=1 \end{vmatrix}$$

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and

## 3. The Convex Spline Interpolant

The data  $\{(t_i, y_i)\}_{i=1}^n$  are called convex if the point  $(t_{i_2}, y_{i_2})$ lies on or beneath the line joining the points  $(t_{i_1}, y_{i_1})$  and  $(t_{i_3}, y_{i_3})$  whenever  $1 \le i_1 < i_2 < i_3 \le n$ . Equivalently,  $[t_{i_1}, t_{i_2}, t_{i_3})f(\cdot) = 0$ 

(where f is any interpolant to the data) or

$$d_{i} = \frac{y_{i+2} - y_{i+1}}{t_{i+2} - t_{i+1}} - \frac{y_{i+1} - y_{i}}{t_{i+1} - t_{i}} \ge 0$$

for i = 1, 2, ..., m(= n-2).

In this chapter we address the problem of finding, for convex data, the smoothest convex interpolant; that is, the convex interpolant having second derivative of minimal norm over all smooth convex interpolants. The natural cubic spline interpolant, the smoothest of all interpolants, regrettably does not always preserve the convexity of the data. In chapter 1 we showed that  $f_*$ , the natural cubic spline interpolant, has second derivative

$$f_{*}^{(2)} = \sum_{j=1}^{m} \alpha_{j} N_{j}$$

where the coefficients  $\alpha_1, \alpha_2, \ldots, \alpha_m$  satisfy (1.13). If any  $\alpha_i$  is negative, then  $f_*$  is actually concave on a subset of [a,b].

Let  $\{(t_i, y_i)\}_{i=1}^n$  denote convex data and let A denote the set of convex interpolants in  $L_2^{(2)}[a,b]$ . We assume that A is nonempty.

(There are convex data for which A is empty. For example, let

 $y_i = |t_i|$  and  $t_1 = -2$ ,  $t_2 = -1$ ,  $t_3 = 0$ ,  $t_4 = 1$ , and  $t_5 = 2$ . The only convex interpolant is f(x) = |x|, which is not in  $L_2^{(2)}[-2,2]$ .)

Using the Peano kernel theorem as we did in chapter 1 we can show that if f  $\epsilon A$  then  $T(f^{(2)}) = \underline{d}$  where  $T:L_2[a,b] \rightarrow R^m$  is given by  $(Tg_i):=(g,N_i)$ . Hence if

$$B = \{g \in L_2[a,b]: g \ge 0 \text{ and } Tg = \underline{d}\},\$$

then problems

Find  $f_* \in A$  such that  $||f_*^{(2)}||_2 \leq ||f^{(2)}||_2$  for all  $f \in A$  (3.1) and

Find  $g_* \in B$  such that  $||g_*||_2 \leq ||g||_2$  for all  $g \in B$  (3.2) are equivalent and the solutions are related via  $g_* = f_*^{(2)}$ . Since B is a nonempty closed convex set, we consider (3.2) as finding the distance from a point to a closed convex set in a Hilbert space.

<u>Proposition</u> ([L, page 69]): Let x be an element of a Hilbert space H and let K be a nonempty closed convex subset of H. Then there exists a unique element  $k_0 \in K$  such that

$$||\mathbf{x} - \mathbf{k}_0|| \le ||\mathbf{x} - \mathbf{k}||$$
 for all  $\mathbf{k} \in \mathbf{K}$ 

 $\underline{Furthermore}, \ k_{0} \ \underline{is \ characterized \ by}$ 

$$(x - k_{o}, k - k_{o}) \leq 0$$
 for all  $k \in K$ .

Since we wish to find the element of minimal norm in B, X corresponds to the zero function and hence  $g_*$  is characterized by

$$(g_*, g-g_*) \ge 0$$
 for all  $g \in B$ . (3.3)

<u>Propostion</u> ([MSSW, proposition 2.1]): If there exist coefficients  $\alpha_1, \alpha_2, \dots, \alpha_m$  satisfying

$$\int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j} N_{j})_{+} N_{i}(t) dt = d_{i} \quad i=1,2,...,m,$$
(3.4)

then  $g_* = (\sum_{j=1}^{m} \alpha_j N_j)_+$ . Furthermore, such coefficients exist if there exists  $\hat{g} \in B$  such that  $\{N_i\}_{i=1}^{m}$  are linearly independent over the support of  $\hat{g}$ .

<u>Proof</u>: Assume  $\alpha_1, \alpha_2, \dots, \alpha_m$  satisfy (3.4). Denote  $s = \sum_{j=1}^{m} \alpha_j N_j$  and assume gEB. Define (h)\_ = (-h)\_+ so that

 $h=(h)_{+}-(h)_{-}.$ 

Then

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$$(s)_{+}, g^{-}(s)_{+})$$

$$= (s + (s)_{-}, g - (s)_{+})$$

$$= (s, g - (s)_{+}) + ((s)_{-}, g - (s)_{+})$$

$$= ((s)_{-}, g) - ((s)_{-}, (s)_{+})$$

$$= ((s)_{-}, g)$$

$$\geq 0.$$

The last inequality is valid since both (s)\_ and g are nonnegative functions. Hence (s)\_ satisfies (3.3).

We now show that we can find coefficients  $\alpha_1, \alpha_2, \dots, \alpha_m$  so that (3.4) holds by following the procedure employed in [MSSW].

We begin by considering the problem

$$\inf \int_{a}^{b_{m}} (\sum_{j=1}^{\infty} \sum_{j=1}^{N} \sum_{j=1}^{N} \sum_{j=1}^{j} (t) dt : \sum_{i=1}^{\infty} \sum_{j=1}^{n} \sum_$$

and showing that if the infimum is attained at some  $\underline{\alpha}$ , then for some positive constant C the coefficients  $C\alpha_1$ ,  $C\alpha_2$ ,...,  $C\alpha_m$  satisfy (3.4).

If the infimum of (3.5) is attained at  $\frac{\alpha}{\alpha}$ , then  $\frac{\alpha}{\alpha}$  is a critical point of the Largrangian

$$L(\underline{\alpha}, \lambda) = \int_{a}^{b} \prod_{j=1}^{m} \sum_{j=1}^{m} \alpha_{j} N_{j} + (t) dt + \lambda (1 - \sum_{j=1}^{m} \alpha_{j} d_{j}). \quad (3.6)$$

At a minimum of L we must have

$$0 = 2 \int_{a}^{b} \sum_{j=1}^{m} \alpha_{j} N_{j} N_{j} N_{i}(t) dt - \lambda d_{i} \quad i=1,2,...,m \quad (3.7)$$

and  $\underline{\alpha} \cdot \underline{d} = 1$  for some  $\lambda$ .

Now multiply (3.7) by  $\boldsymbol{\alpha}_{i}$  and sum over i=1,2,...,m to obtain

$$2\int_{a}^{b} \frac{m}{j=1} \frac{m}{j} \frac{m}{j} \frac{m}{j+1} \frac{(\sum_{i=1}^{m} \alpha_{i} N_{i})(t)dt - \lambda \sum_{i=1}^{m} \alpha_{i} d_{i} = 0}{i=1}$$

or

$$\lambda = 2 \int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j} N_{j})_{+}^{2}(t) dt \ge 0.$$
 (3.8)

If  $\lambda > 0$ , then (3.7) reveals that

$$\int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j}^{*} \dot{N}_{j}) N_{i}(t) dt = d_{i} \quad i=1,2,\dots,m \quad (3.9)$$

where  $\alpha_{j}^{*} = 2 \alpha_{j} / \lambda$ . If  $\lambda = 0$ , then (3.8) reveals that

$$\int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j} N_{j})_{+}(t) dt = 0$$

where  $\underline{\alpha} \cdot \underline{d} = 1$ . This implies that  $(\sum_{j=1}^{m} \alpha_{j} N_{j}) \leq 0$ . However, for any j=1

g  $\varepsilon$  B we have

$$\int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j} N_{j}) g(t) dt = \sum_{j=1}^{m} \alpha_{j} (N_{j}, g)$$
$$= \sum_{i=1}^{m} \alpha_{i} d_{j}$$

= 1

which is impossible because g is nonnegative on [a,b]. We conclude that  $\lambda$  is strictly positive and, if the infimum in (3.5) is attained by some  $\underline{\alpha}$ , that (3.4) is solvable. We now show that the infimum is attained.

Let  $\{\underline{\alpha}^{(k)}\}_{k=1}^{\infty}$  be a minimizing sequence. If  $\{\|\underline{\alpha}^{(k)}\|\}_{k=1}^{\infty}$  is unbounded, then divide the objective function of (3.6) by  $\|\underline{\alpha}\|_{\infty}^2$  and the constraint by  $\|\underline{\alpha}\|_{\infty}$ . There then exists  $\underline{\alpha}$  such that

$$\| \underline{\alpha} \|_{\infty} = 1,$$

$$\underline{\alpha} \cdot \underline{d} = 0, \text{ and}$$

$$\int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j} N_{j})_{+}^{2} (t) dt = 0.$$
We conclude that  $\sum_{j=1}^{m} \alpha_{j} N_{j}$  is nonpositive, but not identically zero. Since we have assumed there exists  $\hat{g} \in B$  such that the B-splines are linearly independent on the support of  $\hat{g}$ ,

$$0 = \sum_{j=1}^{m} \alpha_j d_j = \sum_{j=1}^{m} \alpha_j (\hat{g}, N_j)$$
$$= (\hat{g}, \sum_{j=1}^{m} \alpha_j N_j)$$
$$< 0$$

which is a contradiction. Hence a minimizing sequence must be bounded and the infimum is attained via a convergent subsequence. This completes the proof of the proposition.

We note that the existence of  $\hat{g} \in B$ , such that  $\{N_i\}_{i=1}^m$  are linearly independent over the support of  $\hat{g}$ , in the previous proposition is guaranteed if  $d_i > 0$  for each i. Then each  $g \in B$  must be positive on some subinterval of  $[t_i, t_{i+2}]$ , the support of  $N_i$ , for each i.

Now we consider the implication of allowing  $d_k = 0$  for some k. As a specific example let  $t_i = (i-1)$  for i=1,2,3,4 and let  $\underline{d} = (1,0)^T$ . If  $g_*$  is the positive part of a linear combination of B-splines, then there must exist numbers  $\alpha_1$  and  $\alpha_2$  satisfying

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$$\int_{0}^{3} (\alpha_{1}N_{1} + \alpha_{2}N_{2})_{+}N_{i}(t)dt = \begin{cases} 1 & \text{if } i=1 \\ 0 & \text{if } i=2 \end{cases}$$
(3.10)

which implies that  $\alpha_2 = -\infty$ . This is equivalent to the solution being identically zero on [1,3]. In fact, any g  $\epsilon$  B must be of the form g = g  $\chi_{[0,1]}$ . It is shown in [MSSW, theorem 3.1] that the solution to (3.2) is

$$g_* = \left(\sum_{j=1}^{m} \alpha_j N_j\right)_{+} \chi_{\Gamma}$$

for appropriate coefficients  $\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\ldots,\boldsymbol{\alpha}_m$  where

$$\Gamma: = [a,b]/\{\bigcup_{j=1}^{m} (t_j,t_{j+2}) : d_j = 0\}.$$

Hence the solution to (3.2) with  $t_i = (i-1)$  for i=1,2,3,4 and  $\underline{d} = (1,0)^T$  is

$$g_* = 3N_1 X[0,1].$$

Unless otherwise stated we assume  $d_i > 0$  for each i for the remainder of this chapter.

Before we consider how to compute the coefficients  $\alpha_1, \alpha_2, \ldots, \alpha_m$ which satisfy (3.4), we give a procedure for integrating  $g_*$ . Define  $\beta_i$ ,  $\Delta\beta_i$ ,  $\Delta t_i$ , and  $\Delta y_i$  as in chapter 1. We integrate  $g_*$  on each subinterval  $[t_i, t_{i+1}]$  separately, forming a piecewise polynomial, by solving the differential equation

$$p_{*i}^{(2)}(t) = (\beta_{i} + \frac{\Delta \beta_{i}}{\Delta t_{i}}(t-t_{i}))_{+}$$
(3.11)

for  $t_i \leq t \leq t_{i+1}$  with boundary conditions  $p_*(t_i) = y_i$  and  $p_*(t_{i+1}) = y_{i+1}$ .

Two integrations gives us

$$p_{*i}^{(1)}(t) = \frac{\Delta t_{i}}{2\Delta\beta_{i}} (\beta_{i} + \frac{\Delta\beta_{i}}{\Delta t_{i}} (t-t_{i}))_{+}^{2} + c_{i}$$
(3.12)

and

$$p_{*i}(t) = \frac{\Delta t_{i}}{6(\Delta \beta_{i})^{2}} (\beta_{i} + \Delta \beta_{i}(t-t_{i}))^{3}_{+} + c_{i}(t-t_{i}) + e_{i}$$
(3.13)

for constants c<sub>i</sub> and e<sub>i</sub>. We proceed by cases.

Case 1 occurs when both  $\beta_i$  and  $\beta_{i+1}$  are nonnegative. The nonnegativity constraint is not active in this case and so (3.13) is equivalent to (1.16), although with modified constants  $c_i$  and  $e_i$ . The values  $p_{*i}^{(j)}(t_i)$  for j = 0,1,2,3, are given by (1.18).

Case 2 occurs when  $\beta_i < 0$  and  $\beta_{i+1} > 0$ . In this case  $p_{*i}$  can be defined by two polynomials: a linear polynomial  $q_{i1}$  defined on  $[t_i, \tau_i]$  - where the nonnegativity constraint is active and hence the second derivative is zero - and a cubic polynomial defined on  $[\tau_i, t_{i+1}]$  where

$$\tau_{i} = t_{i} - \beta_{i} \Delta t_{i} / \Delta \beta_{i}$$
(3.14)

Applying the boundary condition  $p_{*i}(t_i) = y_i$  we obtain  $e_i = y_i$ . Applying  $p_{*i}(t_{i+1}) = y_{i+1}$  we get an equation for  $c_i$ :

$$\frac{(\Delta t_{i})^{2}}{6(\Delta \beta_{i})^{2}}(\beta_{i+1})^{3} + c_{i}\Delta t_{i} + y_{i} = y_{i+1}.$$

Solving for  $c_i$  we have

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$$c_{i} = \frac{\Delta y_{i}}{\Delta t_{i}} - \frac{(\beta_{i+1})^{3} \Delta t_{i}}{2(\Delta \beta_{i})^{2}}$$
(3.15)

From (3.11), (3.12), and (3.13) we obtain

$$q_{i1}(t_{i}) = y_{i}$$

$$q_{i1}^{(1)}(t_{i}) = c_{i}$$

$$q_{i1}^{(2)}(t_{i}) = 0$$

$$q_{i1}^{(3)}(t_{i}) = 0$$
(3.16)
$$q_{i2}(\tau_{i}) = c_{i}(\tau_{i} - t_{i}) + y_{i}$$

$$q_{i2}^{(1)}(\tau_{i}) = c_{i}$$

$$q_{i2}^{(2)}(\tau_{i}) = 0$$

$$q_{i2}^{(3)}(\tau_{i}) = \Delta\beta_{i}/\Delta t_{i}$$

where  $\tau_{\underline{i}}$  and  $c_{\underline{i}}$  are given by (3.14) and (3.15) respectively.

Case 3 occurs when  $\beta_i > 0$  and  $\beta_{i+1} < 0$ . In this case  $p_{*i}$  is defined by a cubic polynomial  $q_{i1}$  on  $[t_i, \tau_i]$  and by a linear polynomial  $q_{i2}$  on  $[\tau_i, t_{i+1}]$  with  $\tau_i$  defined by (3.14). These polynomials are determined by the values

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$$q_{i1}(t_{i}) = y_{i}$$

$$q_{i1}^{(1)}(t_{i}) = c_{i} + (\beta_{i})^{2} \Delta t_{i} / (2\Delta \beta_{i})$$

$$q_{i1}^{(2)}(t_{i}) = \beta_{i}$$

$$q_{i1}^{(3)}(t_{i}) = \Delta \beta_{i} / \Delta t_{i}$$

$$q_{i2}(\tau_{i}) = c_{i}(\tau_{i} - t_{i}) + e_{i}$$

$$q_{i2}^{(1)}(\tau_{i}) = c_{i}$$

$$q_{i2}^{(2)}(\tau_{i}) = 0$$

$$q_{i2}^{(3)}(\tau_{i}) = 0$$

where  $\mathbf{c}_{\mathbf{i}}$  and  $\mathbf{e}_{\mathbf{i}}$  are given by

$$c_{i} = \frac{\Delta y_{i}}{\Delta t_{i}} - \frac{(\beta_{i})^{3} \Delta t_{i}}{2(\Delta \beta_{i})^{2}}.$$

and

$$e_{i} = y_{i} - \frac{(\beta_{i})^{3}(\Delta t_{i})^{2}}{6(\Delta \beta_{i})^{2}}$$
.

Case 4 occurs when  $\beta_i$  and  $\beta_{i+1}$  are both nonpositive. In this case we obtain a linear polynomial defined on  $[t_i, t_{i+1}]$  and determined by

$$p_{*i}(t_{i}) = y_{i}$$

$$p_{*i}^{(1)}(t_{i}) = \Delta y_{i} / \Delta t_{i}$$

$$p_{*i}^{(2)}(t_{i}) = 0$$

$$p_{*i}^{(3)}(t_{i}) = 0.$$
(3.18)

Since  $g_*$  is piecewise linear and continuous (with knots at the  $t_i$ 's and  $\tau_i$ 's),  $f_*$  will be piecewise cubic with two continuous derivatives (if  $d_i > 0$  for each i). We call  $f_*$  the convex cubic spline interpolant.

Now we turn our attention to the task of numerically calculating the coefficients  $\alpha_1, \alpha_2, \ldots, \alpha_m$  which satisfy (3.4). We continue to assume that  $d_i > 0$  for each i. Define  $F: \mathbb{R}^m \to \mathbb{R}^m$  by  $F = (F_1, F_2, \ldots, F_m)^T$ where

$$F_{i}(\underline{\alpha}) = \int_{a}^{b} \sum_{j=1}^{m} \alpha_{j} N_{j} + N_{i}(t) dt \quad i=1,2,\ldots,m. \quad (3.19)$$

We wish to solve  $F(\underline{x}) = \underline{d}$ .

One method is to use Jacobi iteration. An initial guess  $\underline{x}^{(o)} = (x_1^{(o)}, x_2^{(o)}, \dots, x_m^{(o)})^T$  is chosen and a sequence  $\{\underline{x}^{(k)}\}_{k=0}^{\infty}$  is generated by calculating  $\underline{x}^{(k+1)}$ , once  $\underline{x}^{(k)}$  is known, by solving

$$F_{i}(x_{1}^{(k)},...,x_{i-1}^{(k)},x_{i}^{(k+1)},x_{i+1}^{(k)},...,x_{m}^{(k)}) = d_{i}$$
for  $x_i^{(k+1)}$  for each i. A modification, the Gauss-Seidel iteration, involves calculating  $\underline{x}^{(k+1)}$ , once  $\underline{x}^{(k)}$  is known, by solving

$$F_{i}(x_{1}^{(k+1)}, \dots, x_{i-1}^{(k+1)}, x_{i}^{(k+1)}, x_{i+1}^{(k)}, \dots, x_{m}^{(k)}) = d_{i}$$

for  $x_i^{(k+1)}$  for i=1,2,...,m in succession. Both Jacobi and Gauss-Siedel iterations converge globally as proved in [IMS]

Now we consider Newton's method to solve  $G(\underline{x}) = F(\underline{x}) - \underline{d} = \theta$ . We pick a suitable initial guess  $\underline{x}^{(0)}$  and form a sequence  $\{\underline{x}^{(k)}\}_{k=0}^{\infty}$  by solving

$$(\nabla G)(\underline{x}^{(k)})(\underline{x}^{(k+1)} - \underline{x}^{(k)}) = -G(\underline{x}^{(k)})$$
(3.20)

for  $\underline{x}^{(k+1)}$  once  $\underline{x}^{(k)}$  is known. Since  $\nabla G = \nabla F$ , we can express (3.20) alternately as

$$(\nabla F)(\underline{x}^{(k)})(\underline{x}^{(k+1)}) - \underline{x}^{(k)}) = \underline{d} - F(\underline{x}^{(k)}).$$
(3.21)

The entries of the Jabocian matrix F are

$$(\nabla F)_{ij}(\underline{\alpha}) = \int_{a}^{b} (\sum_{k=1}^{m} \alpha_{k} N_{k})^{o} N_{j} N_{i}(t) dt \qquad (3.22)$$

where  $(\sum_{k=1}^{m} \alpha_k N_k)^{o}_{+}$  is the characteristic function for the support of k=1

 $(\sum_{j=1}^{m} \alpha_{j}N_{j})_{+}$ . We see that  $\nabla F$  is symmetric and tridiagonal at each  $\underline{\alpha}$ . j=1 j = 1 j = 1. We now characterize those  $\underline{\alpha}$  for which  $(\nabla F)(\alpha)$  is positive definite.

Lemma (3.1): The Jacobian  $(\nabla f)(\alpha)$  is positive definite if and only if

 $\begin{pmatrix} m \\ \Sigma \\ k=1 \end{pmatrix}^{m} \left( \sum_{k=1}^{m} \alpha_{k} N_{k} \right)_{+} \frac{\text{does not vanish identically on any of the subintervals}}{[t_{i}, t_{i+2}] \text{ for } i=1,2,\ldots,m}.$ 

<u>Proof</u>: For any  $\underline{x} \in K^m$  we have

$$\underline{x}^{\mathrm{T}}(\nabla F)(\underline{\alpha})\underline{x} = \sum_{i=1}^{m} x_{i} \sum_{j=1}^{m} (\nabla F)_{ij}(\underline{\alpha})x_{j}$$
$$= \int_{a}^{b} (\sum_{k=1}^{m} \alpha_{k}N_{k})_{+}^{o} (\sum_{j=1}^{m} x_{j}N_{j}) (\sum_{i=1}^{m} x_{i}N_{i})(t)dt$$
$$= \int_{a}^{b} (\sum_{k=1}^{m} \alpha_{k}N_{k})_{+}^{o} (\sum_{i=1}^{m} x_{i}N_{i})^{2}(t)dt$$
$$\geq 0$$

If  $(\sum \alpha_{i} \alpha_{j})_{j+1}$  does not vanish identically on  $[t_{i}, t_{i+2}]$  for each i, then equality holds if and only if  $x_{i} = 0$  for each i. If there exists some k such that  $(\sum_{j=1}^{m} \alpha_{j} N_{j})_{+}$  is identically zero on  $[t_{k}, t_{k+2}]$ , then equality does hold for the nonzero vector  $\underline{x}$  defined by  $x_{i} = \delta_{ik}$ for each i. This completes the proof of the lemma.

From (3.20) we see that

$$F_{i}(\underline{\alpha}) = \sum_{j=1}^{m} \alpha_{j} \int_{a}^{b} (\sum_{k=1}^{m} \alpha_{k} N_{k})^{o}_{+} N_{j} N_{i}(t) dt$$
$$= \sum_{j=1}^{m} \alpha_{j} (\nabla F)_{ij}(\underline{a})$$

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so that  $F(\underline{\alpha}) = (\nabla F)(\underline{\alpha}) \underline{\alpha}$ . Newton's method - equation (3.22) - takes the form

$$(\nabla F)(\underline{x}^{(k)})\underline{x}^{(k+1)} = \underline{d}.$$
 (3.23)

<u>Theorem (3.2)</u>: If  $(\nabla F)(\underline{x}^{(k)})$  is positive definite, then  $(\nabla F)(\underline{x}^{(k+1)})$ is positive definite for each k and, hence, Newton's method - equation 3.23) - is always well-defined.

<u>Proof</u>: Having the known values  $x_i^{(k)}$ , we wish to determine the values  $x_i^{(k+1)}$  satisfying

$$\int_{S(k)} (\sum_{j=1}^{m} x_j^{(k+1)} N_j) N_i(t) dt = d_i \quad i=1,2,\dots,m \quad (3.24)$$

where S(k) is the support of  $(\sum_{j=1}^{m} x_j^{(k)} N_j)_+$ . Since  $(\nabla F)(\underline{x}^{(k)})$  is positive definite, then S(k)  $\bigcup [t_i, t_{i+2}]$  contains an interval for each i. Since  $d_i > 0$ , then  $(\sum_{j=1}^{m} x_j^{(k+1)} N_j)_+$  is positive on some subinterval of  $[t_i, t_{i+2}]$ . Hence,  $(\nabla F)(\underline{x}^{(k+1)})$  is positive definite. This completes the proof of the Theorem.

Note that if  $\underline{x}^{(0)}$  has all positive components (for example, if  $x_i^{(0)} = 1$  for each i, then S(0) = [a,b] and  $\sum_{j=1}^{m} x_j^{(1)} N_j$  is the second derivative of the natural cubic spline interpolant.

Now we assume that  $d_k = 0$  for some k. In this case special care must be exercised since  $\{x_k^{(j)}\}_{j=0}^{\infty}$  may diverge to  $-\infty$ , preventing any numerical convergence. We already know that  $d_k = 0$  implies that the data points  $(t_k, y_k)$ ,  $(t_{k+1}, y_{k+1})$ , and  $(t_{k+2}, y_{k+2})$  are collinear and, hence, any convex interpolant must be linear on  $[t_k, t_{k+2}]$ . Equivalently, the second derivative of any convex interpolant must be zero on  $[t_k, t_{k+2}]$ . Hence  $g_*$  is of the form

$$(\sum_{j=1}^{m} x_j N_j)_{+} \{\chi_{[a,t_k]} + \chi_{[t_{k+2},b]}\}.$$

Since the value of  $x_k$  is immaterial and the k-th equation is automatically satisfied, the number of equations and unknowns each reduce by one. For computational convencience (3.23) can still be used with the following modifications:  $(\nabla F)_{kk} = 1$ ,  $(\nabla F)_{k,k+1} = 0$ , and  $(\nabla F)_{k,k+1} = 0$ .

If  $d_k = 0$ , then the solution is discontinuous at  $t_k$  if  $x_{k-1} > 0$ and is discontinuous at  $t_{k+2}$  if  $x_{k+1} > 0$ . If the solution is discontinuous, then  $f_*$  will have only one continuous derivative.

A further problem is encountered when  $d_{k-1}$  and  $d_{k+1}$  are both zero, but  $d_k$  is nonzero for some k. Any nonnegative function g which satisfies the (k-1)-st and (k+1)-st equations can not satisfy the k-th equation since g is identically zero on  $[t_{k-1}, t_{k+1}]$  and on  $(t_{k+1}, t_{k+2}]$ . We conclude that there does not exist any convex interpolant in  $L_2^{(2)}[a,b]$  (and no solution to the problem as posed). However, we can find a convex interpolant whose second derivative is of the form

$$(\sum_{j=1}^{m} x_{j} N_{j})_{+} \{ \chi_{[a,t_{k-1}]} + \chi_{[t_{k+3},b]} \}$$

satisfying all but the k-th equation. We already know that this convex interpolant must be linear on  $[t_{k-1}, t_{k+1}]$  and on  $[t_{k+1}, t_{k+3}]$  and, hence, piecewise linear on  $[t_{k-1}, t_{k+3}]$ . If  $d_k$  is nonzero, then there will be a discontinuity in slope at  $t_{k+1}$ . For the convenience of utilizing (3.23) we can set  $d_k$  to be zero to satisfy the k-th equation. The discontinuity in slope will show up after we integrate the solution to obtain the interpolant.

Figure (3.1) displays the natural cubic spline interpolant to the function

$$f(t) = \frac{1}{(0.05+t)(1.05-t)}$$

at the knots  $t_1 = 0$ ,  $t_2 = 0.1$ ,  $t_3 = 0.4$ ,  $t_4 = 0.7$ ,  $t_5 = 0.8$ , and  $t_6 = 1.0$ . Figure (3.2) displays the convex spline interpolant to this function. Table (3.1) shows the convergence results for Jacobi, Gauss-Seidel, and Newton's method iterations taken from [IMS]. Note the quadratic convergence characteristic of Newton's method. These convergence results are typical.



Figure (3.1): The Natural Cubic Spline Interpolant.



Figure (3.2): The Convex Cubic Spline Interpolant

	F(x <sup>(r</sup>	1)) - d    2	
Iteration Number	Jacobi	Gauss Seidel	Newton
1	.46 x $10^2$	.27 x $10^2$	.19 x $10^2$
2	$.28 \times 10^2$	.11 x 10 <sup>2</sup>	.85 x $60^{1}$
3	.75 x $10^{1}$	.42 x 10 <sup>1</sup>	,29 x 10 <sup>1</sup>
4	.12 x $10^2$	.18 x 10 <sup>1</sup>	.49 x 10 <sup>0</sup>
5	.26 x $10^{1}$	.75 x 10 <sup>0</sup>	.14 x $10^{-1}$
6	.49 x $10^{1}$	.31 x 10 <sup>0</sup>	.11 x $10^{-4}$
7	.10 x 10 <sup>1</sup>	.13 x 10 <sup>0</sup>	.71 x $10^{-11}$
8	.21 x $10^{1}$	$.55 \times 10^{-1}$	.49 x $10^{-12}$
9	.43 x $10^{0}$	.23 x $10^{-1}$	
10	.86 x 10 <sup>0</sup>	$.96 \times 10^{-2}$	
20	.11 x $10^{-1}$	$.16 \times 10^{-5}$	
30	$.14 \times 10^{-3}$	$.26 \times 10^{-9}$	
40	.18 x 10 <sup>-5</sup>	$.58 \times 10^{-13}$	
50	.24 x $10^{-7}$		
60	.30 x $10^{-9}$		
70	$.39 \times 10^{-11}$		

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#### 4. The Shape-Preserving Spline Interpolant

We addressed in chapter 3 the problem of finding, for convex data, the smoothest convex interpolant. We begin this chapter by considering the problem of finding, for concave data, the smoothest concave interpolant. Then we continue the chapter by examining the problem of finding, for general data, the smoothest interpolant which is locally convex where the data are locally convex and is locally concave where the data are locally concave.

Let  $\{(t_i, y_i)\}_{i=1}^n$  denote concave data and let A denote the set of all concave interpolants in  $L_2^{(2)}[a,b]$ . Assume A is nonempty. Using the Peano kernel theorem as we did in chapter 1, we see that, if  $f \in A$ , then

$$\int_{a}^{b} f^{(2)}(t) N_{i}(t) dt = d_{i} \qquad i=1,2,\ldots,m(=n-2)$$

Equivalently, we have  $T(f^{(2)}) = \underline{d}$ . Defining

B: = {g 
$$\varepsilon L_2[a,b]$$
 : g  $\leq 0$  and Tg = d},

we conclude that the problems

Find  $f_* \in A$  such that  $\|f_*^{(2)}\|_2 \leq \|f^{(2)}\|_2$  for all  $f \in A$  (4.1)

(the problem of finding the smoothest concave interpolant) and

Find 
$$g_* \in B$$
 such that  $||g_*||_2 \leq ||g||_2$  for all  $g \in B$ 

are equivalent and the solutions are related via  $g_* = f_*^{(2)}$ .

Of course, the smoothest concave interpolant to the concave data  $\{(t_i, y_i)\}_{i=1}^n$  is the negative of the smoothest convex interpolant to the convex data  $\{(t_i, -y_i)\}_{i=1}^n$ . We highlight this with the following proposition.

<u>Proposition</u> [MSSW]: If there exist coefficients  $\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_m$ satisfying

$$\int_{a}^{b} (\sum_{j=1}^{m} \alpha_{j} N_{j}) N_{i}(t) dt = d_{i} \quad i=1,2,...,m \quad (4.3)$$

<u>then</u>  $g_* = -\left(\sum_{j=1}^{m} \alpha_j N_j\right)_{j=1}$ . <u>Furthermore, such coefficients exist if there</u> <u>exists</u>  $\hat{g} \in B$  <u>such that</u>  $\{N_i\}_{i=1}^{m}$  <u>are linearly independent over the</u> <u>support of</u>  $\hat{g}$ .

We note that the existence of  $\hat{g} \in B$ , such that  $\{N_i\}_{i=1}^m$  are linearly independent over the support of  $\hat{g}$ , in the previous proposition is guaranteed if  $d_i < 0$  for each i. Then each  $g \in B$  is negative on some subinterval of  $[t_i, t_{i+2}]$ , the support for  $N_i$ , for each i.

Now we consider the problem of finding, for general data, a smooth shape-preserving interpolant - a smooth interpolant which is locally convex where the data are locally convex and is locally concave where the data are locally concave. Assuming for the moment that  $d_i$ is nonzero for each i, we define the sets

$$\begin{split} \mathbf{T}_{1} &:= \{ [\mathbf{t}_{i}, \mathbf{t}_{i+2}] : \mathbf{d}_{i} > 0 \} , \\ \mathbf{T}_{2} &:= \{ [\mathbf{t}_{i}, \mathbf{t}_{i+2}] : \mathbf{d}_{i} > 0 \} , \\ \mathbf{\Omega}_{1} &:= \mathbf{T}_{1} / \mathbf{T}_{2} , \\ \mathbf{\Omega}_{2} &:= \mathbf{T}_{2} / \mathbf{T}_{1} , \\ \mathbf{\Omega}_{3} &:= [\mathbf{a}, \mathbf{b}] / (\mathbf{\Omega}_{1} \mathbf{U} \mathbf{\Omega}_{2}) . \end{split}$$

and

Now we define the sets

A: = { f 
$$\varepsilon L_2^{(2)}[a,b]$$
 :  $f^{(2)} \tilde{\chi}_{\Omega_1} \ge 0$  ,  $f^{(2)} \tilde{\chi}_{\Omega_2} \le 0$ ,  
and  $f(t_i) = y_i \quad i=1,2,...,n$  }

(which we assume is nonempty) and

B: = {g 
$$\varepsilon L_2[a,b]$$
 :  $g\chi_{\Omega_1} \ge 0$  ,  $g\chi_{\Omega_2} \le 0$ , and  $Tg = \underline{d}$  }.

We conclude that the problems

•

Find 
$$f_* \in A$$
 such that  $\|f_*^{(2)}\|_2 \leq \|f^{(2)}\|_2$  for all  $f \in A$  (4.4)

and

Find 
$$g_* \in B$$
 such that  $\|g_*\|_2 \le \|g\|_2$  for all  $g \in B$  (4.5)

are equivalent and  $g_* = f_*^{(2)}$ .

The following proposition gives the solution to (4.5). We see that  $f_*\chi_{\Omega_1}$  has the character of the convex spline interpolant,  $f_*\chi_{\Omega_2}$  has the character of the concave spline interpolant, and  $f_*\chi_{\Omega_3}$  has the character of the natural spline interpolant.

<u>Proposition</u> [MSSW]: If there exists coefficients  $\alpha_1, \alpha_2, \dots, \alpha_m$ satisfying

$$\int_{a}^{b} \{ (\sum_{j=1}^{m} \alpha_{j} N_{j})_{+} \chi_{\Omega} - (\sum_{j=1}^{m} \alpha_{j} N_{j})_{-} \chi_{\Omega} \\ + (\sum_{j=1}^{m} \alpha_{j} N_{j}) \chi_{\Omega} \} N_{i}(t) dt = d_{i} \quad i=1,2,...,m$$

$$(4.6)$$

<u>then</u>

$$g_* = \left(\sum_{j=1}^{m} \alpha_j N_j\right)_+ \chi_{\Omega_1} - \left(\sum_{j=1}^{m} \alpha_j N_j\right)_- \chi_{\Omega_2} + \left(\sum_{j=1}^{m} \alpha_j N_j\right) \chi_{\Omega_3}.$$

Furthermore, such coefficients exist if there exists  $\hat{g} \in B$  such that  $\{N_i\}_{i=1}^{m}$  are linearly independent over the support of  $\hat{g}$ .

We note that the existence of  $\hat{g} \in B$ , such that  $\{N\}_{i=1}^{m}$  are linearly independent over the support of  $\hat{g}$ , in the previous proposition is guaranteed if  $d_i$  is nonzero for each i. Then each  $g \in B$  is nonzero on

some subinterval of  $[t_i, t_{i+2}]$ , the support of  $N_i$ , for each i.

We now solve (4.6). Define  $F : \mathbb{R}^m \to \mathbb{R}^m$  where  $F = (F_1, F_2, \dots, F_m)^T$  is given

$$F_{i}(\underline{x}) = \int_{\Omega_{1}} (\sum_{j=1}^{m} x_{j} N_{j})_{+} N_{i}(t) dt$$

$$= \int_{\Omega_{2}} (\sum_{j=1}^{m} x_{j} N_{j})_{-} N_{i}(t) dt$$

$$+ \int_{\Omega_{3}} (\sum_{j=1}^{m} x_{j} N_{j}) N_{i}(t) dt \qquad i=1,2,\dots,m \qquad (4.7)$$

We use Newton's method to solve  $F(\underline{\alpha}) = \underline{d}$ . Picking a suitable initial guess  $\underline{x}^{(0)}$  we produce a sequence  $\{\underline{x}^{(0)}, \underline{x}^{(1)}, \ldots,\}$  by solving

$$(\nabla F)(\underline{x}^{(k)})(\underline{x}^{(k+1)} - \underline{x}^{(k)}) = \underline{d} - F(\underline{x}^{(k)})$$
(4.8)

for  $\underline{x}^{(k+1)}$  once  $\underline{x}^{(k)}$  is known. The Jacobian matrix has entries given by

$$(\nabla F)_{ij}(\underline{\alpha}) = \int_{a}^{b} P(\underline{\alpha})N_{j}(t)N_{i}(t)dt \qquad (4.9)$$

where

$$P(\underline{\alpha}) = \left(\sum_{j=1}^{m} \alpha_{j} N_{j}\right)_{+}^{0} \overline{\chi}_{\Omega_{1}} + \left(\sum_{j=1}^{m} \alpha_{j} N_{j}\right)_{-}^{0} \overline{\chi}_{\Omega_{2}} + \overline{\chi}_{\Omega_{3}}.$$
 (4.10)

From (4.9) we see that  $\nabla\,F$  is symmetric and tridiagonal at each  $\underline{\alpha}$  . We also note that

$$P(\underline{\mathbf{x}}) \begin{pmatrix} \sum_{j=1}^{m} \mathbf{x}_{j} N_{j} \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^{m} \mathbf{x}_{j} N_{j} \end{pmatrix}_{+} \chi_{\Omega_{1}}$$
$$- \begin{pmatrix} \sum_{j=1}^{m} \mathbf{x}_{j} N_{j} \end{pmatrix}_{-} \chi_{\Omega_{2}}$$
$$+ \begin{pmatrix} \sum_{j=1}^{m} \mathbf{x}_{j} N_{j} \end{pmatrix}_{-} \chi_{\Omega_{3}}$$

so that  $F(\underline{x}) = (\nabla F)(\underline{x})\underline{x}$  and, hence, (4.8) reduces to

$$(\nabla F)(\underline{x}^{(k)})\underline{x}^{(k+1)} = \underline{d}.$$
(4.11)

The following lemma (with proof similar to its counterpart in chapter 3) characterizes those  $\underline{\alpha}$  for which  $(\nabla F)(\underline{\alpha})$  is positive definite.

<u>Lemma(4.1)</u>: <u>The Jacobian</u>  $(\nabla F)(\underline{\alpha})$  <u>is positive definite if and only if</u>  $P(\underline{\alpha})$  <u>does not vanish identically on any of the subintervals</u>  $[t_i, t_{i+2}]$  <u>for i=1,2,...,m</u>.

The following theorem is modeled after theorem (3.2).

<u>Theorem (4.2)</u>: If  $(\nabla F)(\underline{x}^{(0)})$  is positive definite, then Newton's method - equation (4.10) - is always well-defined.

Note that if  $\underline{x}^{(0)}$  is given by  $x_i^{(0)} = \text{signum } (d_i)$  for each i, then  $P(\underline{x}^{(0)})$  is the characteristic function for the interval [a,b] and  $\sum_{j=1}^{m} x_j^{(1)} N_j$  is the second derivative of the natural cubic spline interpolant.

If  $d_k = 0$  for some k, then we already know that any shape-preserving interpolant must be linear on  $[t_k, t_{k+2}]$ . In fact any g  $\epsilon$  B must satisfy

$$g = g \{ \chi_{[a,t_k]} + \chi_{[t_{k+2},b]} \}$$
.

The solution in this case is of the form

$$g_* = h \{ \chi_{[a,t_k]} + \chi_{[t_{k+2},b]} \}$$

where

$$\mathbf{h} = \left(\sum_{j=1}^{m} \alpha_{j} N_{j}\right)_{+}^{X} \Omega_{1} - \left(\sum_{j=1}^{m} \alpha_{j} N_{j}\right)_{-}^{X} \Omega_{2} + \left(\sum_{j=1}^{m} \alpha_{j} N_{j}\right)_{-}^{X} \Omega_{3}$$

Since the value of  $\alpha_k$  is immaterial - the k-th equation  $F_k(\underline{\alpha}) = d_k$  of (4.11) being automatically satisfied - the number of equations and unknowns reduce by one each. For computational convenience we can still use (4.10) by setting  $(\nabla F)_{kk} = 1$ ,  $(\nabla F)_{k,k+1} = 0$ , and  $(\nabla F)_{k,k-1} = 0$ .

Once we solve  $F(\underline{\alpha}) = \underline{d}$  we proceed to integrate  $g_{\underline{x}}$  which is piecewise linear (but not necessarily continuous, even if  $d_{\underline{k}}$  is nonzero for each k) to obtain  $f_{\underline{x}}$  which is piecewise cubic. On the interval  $[t_i, t_{i+1}]$   $f_{\underline{x}}$  is given by the solution to the differential equation

$$p_{i}^{(2)}(t) = \beta_{i} + (\Delta \beta_{i} / \Delta t_{i})(t - t_{i})$$
 (4.12)

for  $t_i \leq t \leq t_{i+1}$  if  $[t_i, t_{i+1}] \subset \Omega_3$ ,

$$p_{i}^{(2)}(t) = (\beta_{i} + (\Delta \beta_{i} / \Delta t_{i})(t - t_{i}))_{+}$$
 (4.13)

for  $t_i \leq t \leq t_{i+1}$  if  $[t_i, t_{i+1}] \subset \Omega_1$ , or

$$p_{i}^{(2)}(t) = -(\beta_{i} + (\Delta \beta_{i} / \Delta t_{i})(t - t_{i}))_{-}$$
(4.14)

for  $t_i \leq t \leq t_{i+1}$  if  $[t_i, t_{i+1}] \subset \Omega_2$  with boundary conditions

$$p_i(t_i) = y_i$$
 and  $p_i(t_{i+1}) = y_{i+1}$ .

The function  $p_i$  is either a cubic polynomial or piecewise cubic given by two polynomials  $q_{i1}$  and  $q_{i2}$  defined on separate subintervals of  $[t_i, t_{i+1}]$ . The solution  $p_i$  to (4.11) is given by (1.18). The solution to (4.12) is, depending on signum ( $\beta_i$ ) and signum ( $\beta_{i+1}$ ), given by (1.18), (3.16), (3.17), and (3.18). The solution to (4.13) is determined by (1.18) if  $\beta_i \leq 0$  and  $\beta_{i+1} \leq 0$ , by (3.16) if  $\beta_i > 0$ and  $\beta_{i+1} < 0$ , by (3.17) if  $\beta_i < 0$  and  $\beta_{i+1} > 0$ , and by (3.18) if  $\beta_i \geq 0$  and  $\beta_{i+1} \geq 0$ .

Figures (4.1), (4.3), (4.5) and (4.7) display the natural cubic spline interpolants to the given data. Figures (4.2), (4.4), (4.6), and (4.8) display the corresponding shape-preserving interpolants. Tables (4.1), (4.2), (4.3), and (4.4) give convergence results for Newton's method. Note the quadratic convergence characteristic of Newton's method.

Appendix B lists a FORTRAN program for computing the shape-preserving cubic spline interpolant.

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Figure (4.1): The Natural Cubic Spline Interpolant.



Figure (4.2): The Shape-Preserving Cubic Spline Interpolant.

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Figure:(4.3): The Natural Cubic Spline Interpolant.



Figure (4.4): The Shape-Preserving Cubic Spline Interpolant.

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Figure (4.5): The Natural Cubic Spline Interpolant.



Figure (4.6): The Shape-Preserving Cubic Spline Interpolant.



Figure (4.7): The Natural Cubic Spline Interpolant.



Figure (4.8): The Shape-Preserving Cubic Spline Interpolant.

## Table 4.1

Iteration Number	$\ F(\underline{x}^{(n)}) - \underline{d}\ _2$
1	$0.13 \times 10^{1}$
2	$0.67 \times 10^{0}$
3	$0.25 \times 10^{0}$
4	$0.42 \times 10^{-1}$
5	$0.12 \times 10^{-2}$
6	$0.88 \times 10^{-6}$
7	$0.58 \times 10^{-12}$
8	$0.64 \times 10^{-13}$

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	Tab	le	4.	2
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Iteration N	(umber $  F(\underline{x}^{(n)}) - \underline{d}  _2$
1	$0.12 \times 10^{1}$
2	$0.56 \times 10^{0}$
3	$0121 \times 10^{0}$
4	$0.36 \times 10^{-1}$
5	$0.11 \times 10^{-2}$
6	$0.85 \times 10^{-6}$
7	$0.54 \times 10^{-12}$
8	$0.70 \times 10^{-13}$

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Table 4.0	Tab	le	4.	3
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Iteration	Number	F( <u>x</u> (n))	- <u>d</u>    2
1		0.24 x	10 <sup>1</sup>
2		0.16 x	10 <sup>1</sup>
3		0.12 x	10 <sup>1</sup>
4		0.90 x	10 <sup>0</sup>
5		0.53 x	10 <sup>0</sup>
6		0.20 x	10 <sup>0</sup>
7		0.26 x	10 <sup>-1</sup>
8		0.42 x	10 <sup>-3</sup>
9		0.97 x	10 <sup>-7</sup>
10		0.37 x	10 <sup>-12</sup>
11		0.21 x	10 <sup>-12</sup>

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Table 4	4.	•4
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Iteration Number	$\left\  F(\underline{x}^{(n)} - \underline{d} \right\ _2$
1	$0.29 \times 10^{1}$
2	$0.13 \times 10^{1}$
3	0.50 x 10 <sup>0</sup>
4	0.11 x 10 <sup>0</sup>
5	$0.56 \times 10^{-2}$
6	$0.16 \times 10^{-4}$
7	$0.13 \times 10^{-9}$
8	$0.26 \times 10^{-12}$

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### 5. Constrained Minimization in a Dual Space

Let C be a convex cone in a normed dual space X with predual Y. Assume  $y_1, y_2, \dots, y_n$  are elements of Y and define T:  $X \rightarrow R^n$  by

$$Tx = (x(y_1), x(y_2), \dots, x(y_n))^T$$

Let B: = {x  $\in C$  : Tx = <u>d</u>} for a given vector <u>d</u>. Consider the problem

Find 
$$x_{*} \in B$$
 such that  $||x_{*}|| \leq ||x||$  for all  $x \in B$  (5.1)

of which (1.10), (3.2), and (4.5) are special cases. In this chapter we study existence and characterization of solutions to (5.1). The following lemma gives sufficient conditions for existence of a solution.

Lemma(5.1): If B is nonempty, if C is weak closed, and if Y is separable, then there exists a solution to problem (5.1).

<u>Proof</u>: Let  $\gamma$ : = inf {||x|| :  $x \in C$  and  $Tx = \underline{d}$  }. Let { $x_n$ } be a sequence in C such that

$$Tx_{n} = \underline{d} \tag{5.2}$$

and

$$\|\mathbf{x}_{n}\| \leq \gamma + 1/n \tag{5.3}$$

for each n. Since Y is separable, by Alaoglu's theorem there exists a weak\* convergent subsequence of  $\{x_n\}$  with weak\* limit x. Since C is weak\* closed we have  $x \in C$ , from (5.2) we have Tx = d, and from (5.3) we have  $||x|| \leq \gamma$  (and hence  $||x|| = \gamma$ ). This completes the proof of the lemma.

Throughout this chapter we assume that B is nonempty, C is weak\* closed, and Y is separable. Since  $x_{\star} = \theta$  if  $\underline{d} = \theta$ , we assume also that  $\underline{d} \neq \theta$  . The following proposition gives us sufficient conditions for C being weak\* closed.

# Proposition (5.2): If C is normed closed and if Y is a reflexive space, then C is weak\* closed.

<u>Proof</u>: Assume  $\{x_n\}$  is a sequence in C with weak\* limit x. We want to show that x is in C. We do this by contradiction. If x is not an element of C, then there exists an element y (an element of both the dual and predual of X) which serves to separate x from C in the sense that

 $x_n(y) > K$ 

for each n and

x(y) < K

for some constant K. This implies that

$$\lim_{n \to \infty} x_n(y) \neq x(y)$$

which is a contradiction. Therefore x  $\epsilon$  C and C is weak\* closed. This completes the proof of the proposition.

For  $\gamma > 0$  we define the convex set  $G(\gamma) \subset \mathbb{R}^n$  by

$$G(\gamma): = \{Tx : x \in C \text{ and } || x || \leq \gamma\}.$$

We now show that  $G(\gamma) = YG(1)$  and  $G(\gamma)$  is closed.

<u>Proposition (5.3)</u>: For each  $\gamma > 0$  we have  $G(\gamma) = \gamma G(1)$ .

Proof: By definition

$$G(\gamma) = \{Tx : x \in C \text{ and } ||x|| \leq \gamma\}$$

$$= \{Tx : \frac{x}{\gamma} \in C \text{ and } ||x/\gamma|| \leq 1\}$$

$$= \{T(x/\gamma) : \frac{x}{\gamma} \in C \text{ and } ||x/\gamma|| \leq 1\}$$

$$= \gamma\{Tw : w \in C \text{ and } ||w|| \leq 1\}$$

$$= \gamma G(1).$$

Proposition (5.4): The set G(1) is closed.

<u>Proof</u>: Assume  $\{\underline{z}_n\}$  is a sequence in G(1) which converges to  $\underline{z}$ . We want to show that  $\underline{z}$  is an element of G(1). Equivalently, we want to show that  $x \in C$  exists such that  $||x|| \leq 1$  and  $Tx = \underline{z}$ .

For each n there exists  $x_n \in C$  such that  $||x_n|| \leq 1$  and  $Tx_n = \frac{z}{n}$ . By Alaoglu's theorem there exists a subsequence of  $||x_n||$  which converges weak\* to some  $x \in C$ . Hence  $||x|| \leq 1$  and  $Tx = \underline{z}$ . This completes the proof of the proposition.

We define

$$\gamma^* := \inf\{\gamma : \underline{d} \in G(\gamma)\}.$$
 (5.4)

Equivalently,

$$\gamma^{\star} = \inf\{\gamma : \text{There exists } x \in C \text{ such that}$$
$$Tx = \underline{d} \text{ and } ||x|| \leq \gamma\}$$
$$= \inf\{||x|| : x \in C \text{ and } Tx = \underline{d}\}.$$
(5.5)

By lemma (5.1) we know that there exists  $x_* \in C$  such that  $||x_*|| = \gamma^*$  and  $Tx_* = \underline{d}$ . We call  $x_*$  an interpolant of minimal norm. We now attempt to characterize  $x_*$  via the Hahn-Banach theorem.

We begin by defining a functional  $\rho$  :  $Y \rightarrow R$  by

$$\rho(\mathbf{y}) = \sup \{ \mathbf{x}(\mathbf{y}) : \mathbf{x} \in \mathbb{C} \text{ and } \| \mathbf{x} \| \leq 1 \}.$$

Notice that if C = X (the unconstrained problem), then  $\rho$  is the norm on Y. In general, since we are taking the supremum over a subset of the closed unit ball U in X, we have  $\rho(y) \leq ||y||$  for all  $y \in Y$ . Since  $\theta$  is an element of C, we have  $\rho \geq 0$ . In convex analysis  $\rho$  is called the support functional of the convex set  $\{x \in C : ||x|| \leq 1\}$ .

Since C is weak\* closed, the supremum is attained at some element of  $\{x \in C : ||x|| \leq 1\}$ ; that is, for any  $y \in Y$  there exists an x (a function of y) such that  $x \in C$ ,  $||x|| \leq 1$ , and  $\rho(y) = x(y)$ . In fact we have ||x|| = 1 unless  $x = \theta$ . The following two propositions reveal that  $\rho$  is continuous, subadditive, and positive homogeneous.

## Lemma(5.5): The functional p is continuous.

<u>Proof</u>: Assume  $y_1$  and  $y_2$  are elements of Y and define  $y = y_1 - y_2$ . Let x be the element in {x  $\in C$  :  $||x|| \le 1$ } such that  $\rho(y_2) = x(y_2)$ . Since  $|x(y)| \le ||y||$ , we have

$$x(y_{2}) - ||y|| \leq x(y_{2}) + x(y)$$

or

$$x(y_{2}) - ||y|| \leq x(y_{1}).$$

Therefore,

$$\rho(y_2) - ||y|| \le \rho(y_1).$$

The elements  $y_1$  and  $y_2$  can be interchanged to obtain

$$\rho(y_1) - ||y|| \le \rho(y_2)$$

and hence

$$|\rho(y_1) - \rho(y_2)| \leq ||y_1 - y_2||.$$

Lemma (5.6): The functional  $\rho$  is subadditive and positive homogeneous (hence convex).

<u>Proof</u>: Assume  $y_1$  and  $y_2$  are in Y. To show that  $\rho$  is subadditive we must show that

$$\rho(y_1 + y_2) \leq \rho(y_1) + \rho(y_2).$$

By definition

$$\begin{split} \rho(y_1 + y_2) &= \sup \{ x(y_1 + y_2) : x \in C \text{ and } ||x|| \leq 1 \} \\ &\leq \sup \{ x(y_1) : x \in C \text{ and } ||x|| \leq 1 \} \\ &+ \sup \{ x(y_2) : x \in c \text{ and } ||x|| \leq 1 \} \\ &= \rho(y_1) + \rho(y_2). \end{split}$$

Now assume  $\alpha > 0$  and y  $\epsilon$  Y. To show that  $\rho$  is positive homogeneous we must show that

$$\rho(\alpha y) = \alpha \rho(y).$$

 $\rho(\alpha y) = \sup \{ x(\alpha y) : x \in C \text{ and } ||x|| \leq 1 \}$  $= \alpha \cdot \sup \{ x(y) : x \in C \text{ and } ||x|| \leq 1 \}$  $= \alpha \rho(y).$ 

This completes the proof of the lemma.

As an example we compute p for the case  $C = \{x \in L_p[a,b]: x \ge 0\}$ where  $1 . For an arbitrary element g in <math>L_q[a,b]$ , the predual of  $L_p[a,b]$  where p + q = pq, we have for any  $f \in C$  with  $||f||_p \le 1$  by the Minkowski inequality

$$\int_{a}^{b} f(t)g(t)dt \leq \int_{a}^{b} f(t)g_{+}(t)dt$$

 $\leq \left\| f \right\|_{p} \cdot \left\| g_{+} \right\|_{q}$ 

≦ ||g<sub>+</sub>||<sub>q</sub>.

Assuming  $g_{+} \neq 0$ , let

$$f = (g)_{+}^{q-1} / \| (g)_{+}^{q-1} \|_{p}.$$

Then we have f  $\epsilon$  C,  $|| f ||_p = 1$ , and

$$\int_{a}^{b} f(t)g(t)dt = ||g_{+}||$$

Hence

$$\rho(g) = \sup \left\{ \int_{a}^{b} f(t)g(t)dt : f \in C \text{ and } \|f\|_{p} \leq 1 \right\}$$
$$= \|g_{+}\|_{q}.$$

If 
$$g_{+} = 0$$
, then  $\rho(g) = 0$ .

<u>Lemma(5.7)</u>: For all  $\underline{\alpha} \in \mathbb{R}^n$  we have

$$\sum_{i=1}^{n} \alpha_{i} d_{i} \leq \gamma^{*} \rho(\sum_{i=1}^{n} \alpha_{i} y_{i}).$$
(5.6)

<u>Proof</u>: Since  $\gamma^* = \inf\{\gamma : \underline{d} \in G(\gamma)\}$ , we have  $\underline{d} \in G(\gamma^* + \varepsilon)$  for any  $\varepsilon > 0$ . Hence for every positive integer n there exists  $x_m \in C$ 

such that  $Tx_m = \underline{d}$  and  $||x_m|| \le \gamma^* + 1/m$ . Therefore, for any  $\underline{\alpha} \in \mathbb{R}^n$ 

$$\sum_{i=1}^{n} \alpha_{i} d_{i} = \sum_{i=1}^{n} \alpha_{i} x_{m}(y_{i})$$

$$= x_{m} (\sum_{i=1}^{n} \alpha_{i} y_{i})$$

$$\leq ||x_{m}|| \rho (\sum_{i=1}^{n} \alpha_{i} y_{i})$$

$$\leq (\gamma^{*} + 1/m)\rho (\sum_{i=1}^{n} \alpha_{i} y_{i}).$$

Now let  $m \rightarrow \infty$  to obtain (5.6). This completes the proof of the lemma.

Since we know that  $G(\Upsilon^*)$  is closed from proposition (5.4), we could have used  $x_*$  in place of  $x_m$  in the proof of lemma (5.7). The next lemma states that there exists a nonzero vector  $\underline{\beta} \in \mathbb{R}^n$  such that equality holds in (5.6).

<u>Proposition (5.8)</u>: There exists a vector  $\beta \in \mathbb{R}^n$  such that  $||\beta|| = 1$ and

$$\underline{\beta} \cdot \underline{d} = \gamma^* \left( \sum_{i=1}^n \beta_i y_i \right).$$
 (5.7)

<u>Proof</u>: The vector <u>d</u> is an element of  $G(\gamma^*)$ , but not an element of  $G(\gamma^*-\epsilon)$  for any  $\epsilon > 0$ . Hence the closed convex set  $G(\gamma^*-\epsilon)$  and the

vector  $\underline{d}$  can be strictly separated by a hyperplane. This implies the existence of a nonzero vector  $\underline{\beta}(\varepsilon)$  such that

$$\underline{\beta}(\varepsilon) \cdot \underline{y} < \beta(\varepsilon) \cdot \underline{d}$$

for all  $\underline{y} \in G(\gamma^* - \varepsilon)$  and without loss of generality we may assume that  $||\underline{\beta}(\varepsilon)|| = 1$ . Equivalently, we have

$$\underline{\beta}(\varepsilon) \cdot Tx < \underline{\beta}(\varepsilon) \cdot \underline{d}$$

and by the linearity of T

$$x(\sum_{i=1}^{n}\beta_{i}(\varepsilon)y_{i}) < \underline{\beta}(\varepsilon) \cdot \underline{d}$$

for all x  $\varepsilon$  C such that  $||x|| \leq \gamma^* - \varepsilon$ . Hence we obtain

$$(\gamma^* - \varepsilon)\rho(\sum_{i=1}^n \beta_i(\varepsilon)y_i) < \underline{\beta}(\varepsilon) \cdot \underline{d}$$

We can take the limit as  $\varepsilon \to 0$  to obtain a vector <u>6</u> such that  $||\underline{\beta}|| = 1$  and

$$\gamma^* \rho(\sum_{i=1}^n \beta_i y_i) \leq \underline{\beta} \cdot \underline{d}.$$

We have the reverse inequality from lemma (5.7) and therefore

$$\underline{\beta} \cdot \underline{d} = \gamma^* \rho(\sum_{i=1}^n \beta_i y_i).$$

This completes the proof of the lemma.

Let  $\boldsymbol{\lambda}$  be a linear functional defined on the subspace

$$S:= span(y_1, y_2, \dots, y_n)$$

Ъy

$$\lambda(\sum_{i=1}^{n} \alpha_{i} y_{i}) = \sum_{i=1}^{n} \alpha_{i} d_{i}$$

so that (5.6) can now be written

$$\lambda(y) \leq \gamma \rho(y)$$
 for all  $y \in S$ .

The Hahn-Banach theorem states that there exists an element  $\boldsymbol{w}$  in  $\boldsymbol{X}$  such that

$$w(y) = \lambda(y)$$
 for all  $y \in S$  (5.8)

and

$$w(y) \leq \gamma \rho(y)$$
 for all  $y \in Y$ . (5.9)

<u>Theorem (5.9)</u>: <u>The Hahn-Banach extension</u> w is an interpolant of minimal norm.

<u>Proof</u>: From (5.8) we see that  $Tw = \underline{d}$  so that w interpolates the data. To complete the proof we show that  $w \in C$  and  $||w|| = \gamma^*$ .

We show that w is in C by contradiction. Assume w is not an element of C. Since C is weak\* closed, there exists an element  $y_0$  in Y which strictly separates w from C in the sense that

$$w(y_0) > x(y_0)$$
 for all  $x \in C$ . (5.10)

Since C is a cone we have  $\lambda x \in C$  whenever  $\lambda > 0$  and  $x \in C$ . Hence (5.10) implies

$$0 \ge x(y_0)$$
 for all  $x \in C$  (5.11)

(or  $\rho(y_0) = 0$ ) and

$$w(y_0) > 0.$$
 (5.12)

However, from (5.9) and (5.12) we have

$$0 \le w(y_0) \le \gamma^* \rho(y_0) = 0$$

which is a contradiction. Hence w must be an element of C.
$$\gamma^{*} \leq || w || \tag{5.13}$$

since w  $\epsilon$  B (w  $\epsilon$  C and Tw = <u>d</u>). Because  $\rho$  is bounded above by the norm on Y, (5.9) yields

$$w(y) \leq \gamma^{*} ||y||$$
 for all  $y \in Y$ 

and hence

$$\|\mathbf{w}\| \leq \gamma^*. \tag{5.14}$$

Taken together, (5.13) and (5.14) imply that  $||w|| = \gamma^*$ . This completes the proof of the theorem.

Recall that for a given element  $y_0$  in Y there exists an element  $x_0$  (a function of  $y_0$ ) in C such that  $\rho(y_0) = x(y_0)$ . Furthermore, either  $||x_0|| = 1$  or  $x_0$  is the zero element. The following lemma will lead us to the conclusion that, if  $\rho$  is differentiable at  $y_0$ , then  $\rho'(y_0) = x_0$ .

<u>Lemma (5.10)</u>: Let f be a functional defined on a normed linear space Z. If f is differentiable at  $x_0 \in Z$  and if there exists a linear functional  $\lambda$  such that

$$f(z_0) + \lambda(z-z_0) \leq f(z)$$
(5.15)

for all z in some neighborhood of  $z_0$ , then  $\lambda = (\nabla f)(z_0)$ .

<u>Proof</u>: Let  $z = z_0 + tu$  where t > 0 and  $u \in Z$ . Inequality (5.15) yields

$$\lambda(u) \leq \frac{f(z_0 + tu) - f(z_0)}{t}$$
 (5.16)

Since (5.16) holds for all t > 0 (and sufficiently small) and for all  $u \in Z$ , we have  $\lambda \leq (\nabla f)(z_0)$ . Substituting -u for u in (5.16) yields

$$\lambda(u) \ge \frac{f(z_0 - tu) - f(z_0)}{t}$$
(5.17)

for all t > 0 (and sufficiently small) and for all u  $\varepsilon$  Z. Taken together, (5.16) and (5.17) imply  $\lambda = (\nabla f)(z_0)$ .

<u>Corollary (5.11)</u>: If  $\rho$  is differentiable at  $y_{\rho} \in Y$ , then  $\rho'(y_{\rho}) = x_{\rho}$ .

<u>Proof</u>: Since  $\rho(y_0) = x_0(y_0)$  and  $x_0(y) \le \rho(y)$  for all  $y \in Y$ , we have

$$\rho(y_0) + x_0(y - y_0) \leq \rho(y)$$

for all  $y \in Y$ . By the previous lemma we have  $\rho'(y_0) = x_0$ . This completes the proof of the corollary.

Inequality (5.6) motivates the problem

$$\inf_{\alpha} \{ \begin{array}{c} n \\ \rho(\sum \alpha_{i} y_{i}) : \underline{\alpha} \cdot \underline{d} = 1 \} \\ \alpha \\ i = 1 \end{array} \}$$
(5.18)

Notice that if  $\underline{\alpha}$  is any vector satisfying  $\underline{\alpha} \cdot \underline{d} = 1$  and if  $\underline{x}$  is any element of B, then

$$1 = \sum_{i=1}^{n} \alpha_{i} d_{i} = x(\sum_{i=1}^{n} \alpha_{i} y_{i})$$

$$\leq ||x|| \rho(\sum_{i=1}^{n} \alpha_i y_i)$$

and hence

$$\rho\left(\sum_{i=1}^{n} \alpha_{i} y_{i}\right) \geq \frac{1}{\|x\|}$$

This implies that the infimum is positive (and, in fact, is bounded below by  $(\gamma^*)^{-1}$ . If the infimum is attained at some  $\underline{\alpha}^* \in \mathbb{R}^n$  and if  $\rho$ 

is differentiable at  $\sum_{i=1}^{n} \alpha_{i} y_{i}$ , then we are led to a solution to (5.1) as

the next theorem reveals.

Theorem (5.12): If there exists 
$$\underline{\alpha}^* \in \mathbb{R}^n$$
 such that  $\underline{\alpha}^* \cdot \underline{d} = 1$  and  
 $\rho(\sum_{i=1}^n \alpha_i^* y_i) = \inf\{\rho(\sum_{i=1}^n \alpha_i y_i) : \underline{\alpha} \cdot \underline{d} = 1\}$ 

and if  $\rho$  is differentiable at  $\sum_{i=1}^{n} \alpha_{i}^{*} y_{i}^{*}$ , then

$$\gamma^* \rho' (\sum_{i=1}^n \alpha_i y_i)$$

### is an interpolant of minimal norm.

Proof: Problem (5.18) has Lagrangian

$$L(\underline{\alpha}, \lambda) = \rho(\sum_{i=1}^{n} \alpha_{i} y_{i}) - \lambda(\sum_{i=1}^{n} \alpha_{i} d_{i} - 1).$$
 (5.19)

If there exists a solution  $\underline{\alpha}^*$  to (5.18), then there exists  $\lambda^*$  so that  $(\underline{\alpha}^*, \lambda^*)$  is a stationary point of (5.19). Hence

$$x(y_i) - \lambda^* d_i = 0$$
  $i=1,2,...,n$  (5.20)

where 
$$x = \rho'(\sum_{i=1}^{n} \alpha_i^* y_i)$$
,  $x \in C$ ,  $||x|| = 1$ , and  $\alpha^* \cdot \underline{d} = 1$ .

We first show that  $\lambda^* > 0$ . Multiply (5.20) by  $\alpha_i^*$  and

sum over i to obtain

$$x(\sum_{i=1}^{n} \alpha_{i}^{*} y_{i}) = \lambda \sum_{i=1}^{*} \alpha_{i}^{n} \alpha_{i}^{*} d_{i} = \lambda^{*}.$$

Since  $x = \rho'(\sum_{i=1}^{n} \alpha_i^* y_i)$ , we have

$$x(\sum_{i=1}^{n} \alpha_{i}^{*}y_{i}) = \rho(\sum_{i=1}^{n} \alpha_{i}^{*}y_{i})$$

so that

$$\lambda^* = \rho(\sum_{i=1}^n \alpha_i^* y_i) \ge 0$$

Actually, we know that since the infimum is positive, we have  $\lambda^* > 0$ . We can also show this by contradiction. If  $\lambda^* = 0$ , then

$$x(\sum_{i=1}^{n} \sum_{i=1}^{*} y_{i}) \leq 0 \quad \text{for all } x \in C.$$
 (5.21)

Let s be any interpolant in C. (We know that there exists an interpolant in C since B is nonempty.) Then

$$s(\overset{n}{\underset{i=1}{\overset{*}{\sum}}} \overset{n}{\underset{i=1}{\overset{*}{\sum}}} \overset{n}{\underset{i=1}{\overset{*}{\sum}} \overset{n}{\underset{i=1}{\overset{*}{\sum}}} \overset{n}{\underset{i=1}{\overset{*}{\sum}} \overset{n}{\underset{i=1}{\overset{*}{\sum}} \overset{n}{\underset{i=1}{\overset{*}{\sum}} \overset{n}{\underset{i=1}{\overset{*}{\sum}} \overset{n}{\underset{i=1}{\overset{*}{\underset{i=1}{\overset{*}{\sum}}} \overset{n}{\underset{i=1}{\overset{*}{\underset{i=1}{\overset$$

which contradicts (5.21). Therefore,  $\lambda^* > 0$ . Now we show that  $\lambda^* \gamma^* = 1$ . From (5.20) we see that  $x/\lambda^*$  is an interpolant in C. Hence

 $\gamma^* \leq ||\mathbf{x}|| / \lambda^* = 1/\lambda^*$ 

or

$$\gamma^* \lambda^* \leq 1$$
 (5.22)

Let w be an interpolant of minimal norm satisfying (5.9). Then

$$w(\sum_{i=1}^{n} \alpha_{i} y_{i}) \leq \gamma \rho(\sum_{i=1}^{n} \alpha_{i} y_{i}).$$

Equivalently, we have

$$w(\sum_{i=1}^{n} \alpha_{i}^{*} y_{i}) \leq \gamma^{*} x(\sum_{i=1}^{n} \alpha_{i}^{*} y_{i})$$

which leads to

$$1 \leq \gamma^* \lambda^*. \tag{5.23}$$

Taken together, (5.22) and (5.23) imply

$$1 = \gamma^* \lambda^*.$$

This concludes the proof of the theorem.

We consider now the problem of determining when the infimum is attained in (5.18). From proposition (5.8) we know that there exist a nonzero vector  $\underline{\beta}$  such that

$$0 \leq \underline{\beta} \cdot \underline{d} = \gamma \overset{*}{\rho} ( \overset{n}{\underset{i=1}{\Sigma}} \beta_{i} y_{i} ).$$

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If  $\underline{\beta} \cdot \underline{d} > 0$ , then the infimum is attained in (5.18) at  $\underline{\alpha}^* = \underline{\beta}/(\underline{\beta} \cdot \underline{d})$ .

Proposition (5.13): If d is in the relative interior of

S: = {
$$\underline{r}$$
 :  $r \in G(\gamma)$  for some  $\gamma$  },

then there exists a vector  $\beta$  such that

$$1 = \underline{\beta} \cdot \underline{d} = \gamma^* \rho(\sum_{i=1}^n \beta_i y_i).$$

<u>Proof</u>: We prove by contradiction. Assume that every vector  $\underline{\beta}$  which satisfies

$$\underline{\beta} \cdot \underline{d} = \gamma \rho(\sum_{i=1}^{n} \beta_i y_i)$$

also satisfies  $\underline{\beta} \cdot \underline{d} = 0$ . Without loss of generality it can be assumed that there exists a nonzero vector  $\underline{\beta}$  such that

$$0 = \underline{\beta} \cdot \underline{d} = \gamma^* \rho(\sum_{i=1}^n \beta_i y_i)$$

and

$$\underline{\beta} \cdot \underline{y} \ge 0$$
 for all  $\underline{y} \in G(\underline{\gamma}^*)$ .

In any relative neighborhood of  $\underline{d}$  there is a vector  $\underline{z}$  such that  $\underline{\beta} \cdot \underline{z} < 0$ . If  $\underline{z}$  were an element of S, then there would be an element  $\underline{r}$  in  $G(\gamma^*)$  such that  $\underline{z} = \alpha \underline{r}$  for some  $\alpha > 0$ . However, we would then have

$$\underline{\beta} \cdot \underline{z} = \alpha \underline{\beta} \cdot \underline{r} \ge 0$$

which is a contradiction. Therefore  $\underline{z}$  is not an element of S and  $\underline{d}$  is not in the relative interior of S. This completes the proof of the proposition.

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# <u>Appendix A</u>

# A Program for Constructing the Natural Cubic Spline Interpolant

to Given Data.

•

00001 PROGRAM UNCON(INPUT, OUTPUT, TAPE5=INPUT, TAPE6=OUTPUT) 00002C 000030 WE FORM THE NATURAL CUBIC SPLINE INTERPOLANT. 00004C 00005 INTEGER N, M, J 00006 REAL T(50), F(50), D(50), X(50), A(50), PP(4,50) 00007 REAL AA(50),BB(50),CC(50) 00008C THE ARRAYS (T) AND (F) - EACH OF SIZE M, THE NUMBER 000090 OF DATA. POINTS - CONTAIN THE COMPONENTS OF THE DATA. 00010C 000110 THE DATA FILE IS OF THE FOLLOWING FORM 000120 000130 М · 0001.4C T(1),F(I)000150 T(2),F(2)00016C ٠ 000170 000180 000190 T(M),F(M)000200 WHERE WE ASSUME (T) HAS STRICTLY INCREASING COMPONENTS. 000210 000220 READ(3,\*) M 00023 00024 READ(3,\*) (T(I),F(I), I=1,M) 00025 N = M - 200026C THE ARRAY (D) CONSISTS OF THE SCALED 000270 000280 SECOND DIVIDED DIFFERENCES. 000290 00030 DO 100 I=1,N 00031 D(I) = (F(I+2)-F(I+1))/(T(I+2)-T(I+1))-(F(I+1)-F(I))/(T(I+1)-T(I))00032 С 00033 100 CONTINUE 00034C 00035C THE SECOND DERIVATIVE OF THE NATURAL CUBIC SPLINE 000360 00037C INTERPOLANT IS A LINEAR COMBINATION OF LINEAR B-SPLINES. WE CALCULATE THE CDEFFICIENTS. 000380 000390 000400 00041 AA(1) = 0.000042 BB(1) = (T(3) - T(1))/3.000043 CC(1) = (T(3) - T(2))/6.0DO 200 I=2,N-1 00044 00045 AA(I) = (T(I+1)-T(I))/6.000046 BB(I) = (T(I+2)-T(I))/3.000047 CC(I) = (T(I+2) - T(I+1))/6.000048 200 CONTINUE 00049 AA(N) = (T(N+1) - T(N))/6.000050 BB(N) = (T(N+2) - T(N))/3.0

00051 CC(N) = 0.000052 CALL TRID(AA, BB, CC, D, N) 000530 00054C 00055C 00055 A(1) = 0.000057 A(M) = 0.000058 DO 300 I=2,N+1 00059 A(I) = B(I-1)00060 300 CONTINUE 00061C 000620 000630 NOW WE COMPUTE THE NUMBERS PP(J,I) - THE VALUE 00064C OF THE (J-1)ST DERIVATIVE OF THE NATURAL CUBIC SPLINE INTERPOLANT EVALUATED AT T(I). 000650 00033C 000670 00068 DO 400 K=1,N+1 00069 DF = F(K+1) - F(K)00070 DT = T(K+1) - T(K)IA = A(K+1) - A(K)00071 00072 PP(4,K) = DA/DTPP(3,K) = A(K)00073 00074 PP(2,K) = DF/DT - (A(K)/2. + DA/6.)\*DT 00075 PP(1,K) = F(K)00076 400 CONTINUE 00077 PP(4,M) = 0.000078 PP(3,M) = 0.000079 PP(2,M) = 0.000080 PP(1,M) = F(M)00081C 000820 00083C 00084 DO 500 K=1,M 00085 WRITE(6,450) K,T(K),(PP(I,K), I=1,4) 00086 450 FORMAT(5X, 15, 5F14.6) 00087 500 CONTINUE 000880 000890 WE CREATE A DATA FILE FOR PLOTTING THE (JDER)-TH 000900 DERIVATIVE OF THE NATURAL CUBIC SPLINE INTERPOLANT 000910 BY EVALUATING IT AT (MM) EQUALLY SPACED POINTS, 000920 INCLUDING THE ENDFOINTS. WE ASSUME THAT (JDER) HAS VALUE 0, 1, 2, OR 3. 000930 00094C JDER= 0 00095 00096 MM= 201 00097 CALL DATAFL(T, PP, M, MM, JDER) 00098C 00099 STOP 00100 END

00001 SUBROUTINE DATAFL(TX, PP, LI, MM, JDER) 00002C 000030 WE CREATE A DATA FILE FOR PLOTTING THE (JDER)-TH 00004C DERIVATIVE OF THE PIECEWISE CUBIC POLYNOMIAL. WE 000050 ASSUME (JDER) HAS VALUE 0, 1, 2, DR 3. 00006C 00007 INTEGER LI, MM, JDER 00008 REAL TX(100), PP(4,100) 00009 LEFT = 100010 MMONE= MM - 1 WRITE(4,\*) MM 00011 00012 XE= ( TX(LI)-TX(1) )/FLOAT(MMONE) DO 500 IF=1,MM 00013 00014 XT= TX(1) + XE\*FLOAT(IP-1) 00015C 0001.6C WE FIND THE INTERVAL IN WHICH THE POINT (XT) LIES. 00017C 00018 IF ( LEFT .NE. LI ) THEN 00019 DO 200 IS=LEFT,LI-1 00020 IF ( XT .LT. TX(IS+1) ) GO TO 300 00021 200 CONTINUE 00022 300 CONTINUE 00023 END IF 00024 LEFT= IS 00025C 00026C WE NOW COMPUTE THE VALUE OF THE POLYNOMIAL AT 000270 THE POINT (XT) BY USING MESTED MULTIPLICATION. 000280 00029 H = XT - TX(LEFT)00030 FAC= 4.0 - FLOAT(JDER) YT= 0.0 00031 00032 IIO 400 M=4, JIIER+1,-1 YT= (YT/FAC)\*H + PP(M,LEFT) 00033 FAC= FAC - 1.0 00034 00035 400 CONTINUE 00036 WRITE(4,450) XT,YT 00037 450 FORMAT(F8.4,E18.9) 00038 500 CONTINUE 00039 RETURN 00040 END

00001	SUBROUTINE TRID(SUB,DIAG,SUP,B,N)
00002	INTEGER N,I
00003	REAL B(N),DIAG(N),SUB(N),SUP(N)
00004	IF (N.LE.1) THEN
00005	B(1) = B(1)/DIAG(1)
00006	RETURN
00007	END IF
80000	DO 111 I=2,N
00009	SUB(I)= SUB(I)/DIAG(I-1)
00010	<pre>DIAG(I)= DIAG(I) - SUB(I)*SUP(I-1)</pre>
00011	B(I) = B(I) - SUB(I)*B(I-1)
00012 11	1 CONTINUE
00013	E(N) = B(N)/DIAG(N)
00014	DO 222 I=N-1,1,-1
00015	B(I)= (B(I)-SUP(I)*B(I+1))/DIAG(I)
00016 22	2 CONTINUE
00017	RETURN
00018	END

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# Appendix B

A Program for Constructing the Shape-Preserving Cubic Spline Interpolant to Given Data

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00001	PROGRAM MAIN(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
00002C	
00003C	WE COMPUTE A SHAPE-PRESERVING INTERPOLANT
00004C	TO GIVEN DATA.
00005C	
00006C	
00007C	NOTE ON THE SIZE OF THE ARRAYS:
00008C	THE ARRAYS (T), (F), AND (A) MUST BE OF LENGTH
00009C	AT LEAST M. THE NUMBER OF DATA POINTS. THE
00010C	ARRAY (TX) AND THE SECOND COMPONENT OF THE
00011C	ABRAY (PP) SHOULT BE OF LENGTH 2M. THE ABRAYS
000120	(X). (Y). AND (D) MUST BE OF LENGTH AT LEAST M-2.
000130	THE ARRAY (II) MUST BE DE LENGTH AT LEAST M-1.
000140	THE MART (12) NOOT DE OF EEROM AT EEROF A 14
000110	
00014	PEAL T(50) E(50) V(50) V(50) A(50)
00010	$\mathbf{E} = \mathbf{E} \left[ \mathbf{E} $
00017	$\mathbf{N} = \mathbf{I} \times (\mathbf{I} \cup \mathbf{U}) + \mathbf{I} \times (\mathbf{I} \cup \mathbf{U}) + \mathbf{I} \times (\mathbf{I} \cup \mathbf{I} \cup \mathbf{I}) + \mathbf{I} \times (\mathbf{I} \cup \mathbf{I} \cup \mathbf{I} \cup \mathbf{I}) + \mathbf{I} \times (\mathbf{I} \cup \mathbf{I} \cup \mathbf{I}) + \mathbf{I} \times (\mathbf{I} \cup \mathbf{I} \cup \mathbf{I}) + \mathbf{I}$
00018	IRIEGEN MYNYIIMAAYIYJYIFLAGYMM
00019	COMMON D(30),10(30)
000200	
000210	
000220	
000230	THE ARRAYS (T) AND (F) - EACH OF SIZE M, THE NUMBER
00024C	OF DATA POINTS - CONTAIN THE COMPONENTS OF THE DATA.
000250	THE DATA FILE IS OF THE FOLLOWING FORM
00026C	
00027C	М
00028C	T(1),F(1)
000290	T(2),F(2)
000300	•
000310	•
00032C	•
00033C	T(M),F(M)
00034C	
00035C	WHERE WE ASSUME (T) HAS STRICTLY INCREASING COMPONENTS.
00036C	
00037	READ(3,*) M
00038	READ(3,*) (T(I),F(I), I=1,M)
00039	N= M−2
00040C	<i>.</i>
00041C	(EPS) IS A SMALL POSITIVE NUMBER USED TO TEST FOR
000420	CONVERGENCE IN NEWTON'S METHOD - SUBROUTINE (ZERO).
000430	(ITMAX) IS THE MAXIMUM NUMBER OF ITERATIONS
000440	WHICH WE PERMIT FOR NEWTONS METHOD TO CONVERGE.
000450	mien we remit for newford hemoe to donyender
00044	FPS= 1.0F-8
00047	1TMAY= 25
000490	\$ 1) HIV ~ &Q
000400	THE ARRAY (Y) TO THE KNOT CEDUENCE (T) WITH THE
	ENTROTATE TI ANTI TO THE KIGA SECONDE (17 WITH THE
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00051C 00052 TL = T(1)00053 TR= T(M) 00054 DO 120 I=1,N 00055 X(I) = T(I+1)00056 120 CONTINUE 000570 000580 THE ARRAY (D) CONSISTS OF THE SCALED 000590 SECOND DIVIDED DIFFERENCES. 00060C 00061C IT IS IMPORTANT THAT WE IDENTIFY DIVIDED DIFFERENCES 00032C WHICH ARE ZERO. THIS MEANS THAT WE MUST COMPARE TWO FLOATING-POINT NUMBERS. 000630 TO DO THIS WE ASSUME D(K) IS 00034C ZERO IF D(K) IS SMALL. 000650 XEPS= 1.0 00066 00067 DO 130 J=1,20 00068 XEPS= XEPS/10. 00069 Z=1.0 + XEPS00070 IF ( Z .EQ. 1.0 ) GO TO 135 00071 YEP'S= XEP'S 00072 130 CONTINUE 00073 135 CONTINUE 00074 YEPS= YEPS\*1000. 00075C 00076 IO 140 K=1.N 00077 D(K) = (F(K+2)-F(K+1))/(T(K+2)-T(K+1))С 00078 -(F(K+1)-F(K))/(T(K+1)-T(K))00079 IF ( ABS(D(K)) .LE. YEPS ) D(K) = 0.000080 140 CONTINUE 00081C 000820 000830 THE INITIAL GUESS (Y) FOR NEWTON'S METHOD 00084C WILL YIELD THE SECOND DERIVATIVE OF THE 000850 NATURAL SPLINE SOLUTION, EXCEPT POSSIBLY 000860 WHEN D(K) = 0.0 FOR SOME K. 00087C 00088 DO 145 K=1,N 000890 000900 00091 IF ( D(K) .GT. 0.0 ) THEN 00092 Y(K) = 1.0ELSE 00093 00094 Y(K) = -1.0END IF 00095 00096C 00097C 00098 145 CONTINUE

00101 WRITE(6,150)

00099C 00100C

00102 150	FORMAT(/, ' DATA VALUES ',/)
00103	WRITE(6,160) (D(I), I=1,N)
00104 160	FORMAT(5X,4E12.6)
00105	WRITE(6.170)
00106 170	FORMAT(//)
001070	
001080	
001090	TI(K) = 1 INDICATES THAT THE INTERPOLATING CUNCTION
001070	TS CONSTRATINED TO BE CONNEY ON FIGH DENTITE FORCITOR
001100	AND, UENCE TTO GEORME REDINATIVE TO CONCEDATION
001110	TO DE MONNEGATTHE ON THE INTEDIAL
001120	ID DE RORREDHITVE ON THIS INTERVIET
001136	
001140	TO CONSTRATINET TO BE CONCALE ON ETTEN TARANA
001130	
001160	ARD, MERLE, 115 SELUND DERIVATIVE 15 LUNSTRAINED
001170	TO BE NUNPUSITIVE UN THIS INTERVAL.
001130	
001190	IU(K) = 0 INDICATES THAT THE INTERPOLATING FUNCTION
001200	IS UNCONSTRAINED ON [T(K),T(K+1)].
001210	
00122C	
00123	DO 180 I=1,N-1
00124	ID(I+1) = 0
00125	IF (D(I).GE.0.0 .AND. D(I+1).GE.0.0) ID(I+1)= 1
00126	IF (D(I).LE.O.O .AND. D(I+1).LE.O.O) ID(I+1)= -1
00127 180	CONTINUE
00128	IF ( D(1) .GE. 0.0 ) THEN
00129	III(1) = 1
00130	ELSE
00131	ID(1) = -1
00132	END IF
00133C	
00134	IF ( D(N) .GE. 0.0 ) THEN
00135	ID(N+1) = 1
00136	ELSE
00137	TD(N+1) = -1
00138	END IF
001390	
001400	TE A NONZERO DATA VALUE D(I) LIES BETWEEN TWO
001410	7FRO DATA VALUES $D(T-1)$ AND $D(T+1)$ . THEN $D(T)$
001420	IS TAKEN TO BE ZERD FOR COMPUTATIONAL PURPOSES.
001430	
00144	TID 185 T=2.N-1
00145	IE = (II(I-1), EQ, O, O, AND, II(I+1), EQ, O, O) II(I) = 0.0
00144 195	
00140 100	BERTINDE
001480	SUBBOUTINE (ZEBO) CALCULATES THE DIECEWISE
001400	I TACAD GECOND DEDITIATING OF THE SHADE.
001500	DECCEDITING INTEREDO ANT
001510	LUEDENATKO TIKIEULOFUKI*
001010	
00102	LALL ZERU(I,X,N,LINAX,EPS,IFLAU,IL,IK)

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00153C 00154 A(1) = 0.000155 A(M) = 0.000156 DO 190 I=2,N+1 00157 A(I) = Y(I-1)00158 190 CONTINUE 00159C 00160 WRITE(6,200) 00161 200 FORMAT(/, ' PIECEWISE LINEAR 2ND DERIVATIVE ',/) 00162 WRITE(6,210) (I,T(I),A(I), I=1,M) 00163 210 FORMAT(5X, I5, ' ( ', F14.6, ' , ', F14.6, ' )') 00164 WRITE(6,220) 00165 220 FORMAT(//) 00166C 001670 SUBROUTINE (POLY) INTEGRATES THE RESULT 00168C FROM SUBROUTINE (ZERO). 001690 00170 CALL POLY(A,T,PP,M,F,LI,TX) 001710 00172 WRITE(6,230) 00173 230 FORMAT(/, ' KNOTS AND COEFFICIENTS OF PIECEWISE CUBIC',/) 00174 DO 250 I=1,LI 00175 WRITE(6,240) I,TX(I),(PP(J,I), J=1,4) 00176 240 FORMAT(5X, 15, 5F14.6) 00177 250 CONTINUE 00178 WRITE(6,260) IFLAG 00179 260 FORMAT(/, ' ERROR CODE = ', 15,/) 00180 WRITE(6,270) ITMAX 00181 270 FORMAT(/, ' NUMBER OF ITERATIONS =', 15,) 001820 SUBROUTINE (DATAFL) IS USED TO CREATE A 001830 00184C DATA FILE FOR PLOTTING. WE EVALUATE THE (JDER)-TH DERIVATIVE OF THE PIECEWISE CUBIC 001850 00186C POLYNOMIAL AT MM EQUALLY SPACED POINTS, INCLUDING THE ENDFOINTS TL AND TR. WE 001870 ASSUME (JDER) HAS VALUE 0, 1, 2, OR 3. 00188C 00189C 00190 MM= 201 00191 JDER= 0 00192 CALL DATAFL(TX, PP, LI, MM, JDER) 001930 00194 STOP 00195 END

00002C 00003C 00004 INTEGER N,ITMAX,K,J,LJ,L,IFLAG 0005 REAL A(N),X(N),FX(50),AL,XL,AR,XR,DT,DA,T,W 0006 REAL SUS(50),DIG(50),SUF(50),H(50),SUM1,SUM2 0007 REAL RATID,GLEFT,GRIGH,PS,FNORM1,TL,TR 0008 COMMON D(50),ID(50) 00010C INFUT PARAMETERS: 00011C 00012C AINITIAL ESTIMATE FOR NEWTON'S METHOD. 00013C 00014C XKNDT SEQUENCE WITH THE ENDPOINTS DELETED. 00015C 00014C NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS. 00015C 00016C ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD. 00017C 00018C ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD. 00017C 00020C EPSPARAMETER USED TO TEST FOR CONVERGENCE. 00021C TL,TRLEFT- AND RIGHT-ENDPOINTS OF THE 00022C TL,TRLEFT- AND RIGHT-ENDPOINTS OF THE 00022C OUTPUT PARAMETERS: 00022C OUTPUT PARAMETERS: 00022C OUTPUT PARAMETERS: 00022C ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S 00030C METHOD TO CONVERGENCE INDICATED BY COMPARING 00032C IFLAGIFLAGE 1: CONVERGENCE INDICATED BY COMPARING 00032C IFLAGIFLAGE 1: CONVERGENCE INDICATED BY COMPARING 00033C THE L1 NORMS OF THE ITERATIONS EXCEEDED ITMAX. 00033C C (UNDERGE OF ITERATIONS EXCEEDED ITMAX. 00033C C (UNDERGENCE INDICATED BY COMPARING 00034 C IFLAGE 2: NUMBER OF ITERATIONS EXCEEDED ITMAX. 00035 C (UNDERGENCE INDICATED BY COMPARING 00037 DO FORMAT(' ITERATION NUMBER AND RESIDUAL:',/ 00038 C (UNDERMET(CONVERGENCE IS EXPECTED.',/) 0039 DO 350 LJ=1,ITHAX 00040C THE ARRAYS (SUB), (DIAB), AND (SUP) CONTAIN 00041C THE ARRAYS (SUB), (DIAB), AND (SUP) CONTAIN 00042C THE SUMMETRY OF THE TRIDIAGONAL POSITIVE-DEFINITE 00433C JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A). 0044C IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER, 0044C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 0044C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 0044C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 0044C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 0044C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 0044C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 004	00001	SUBROUTINE ZERD(A,X,N,ITMAX,EPS,IFLAG,TL,TR)
00003C 00004 INTEGER N,ITMAX,K,J,LJ,L,IFLAG 00005 REAL A(N),X(N),FX(50),AL,XL,AK,XR,DT,DA,T,W 00006 REAL SUB(50),DIAG(50),SUP(50),H(50),SUM1,SUM2 00007 REAL RATIO,GLEFT,GRIGH,EFS,FNORM1,TL,TR 00008 COMMON D(50),ID(50) 00007C 00010C INPUT PARAMETERS: 00011C AINITIAL ESTIMATE FOR NEWTON'S METHOD. 00013C AINITIAL ESTIMATE FOR NEWTON'S METHOD. 00014C XKNOT SEQUENCE WITH THE ENDPOINTS DELETED. 00015C NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS. 00017C 00016C NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS. 00017C 00018C ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD. 00019C EPSPARAMETER USED TO TEST FOR CONVERGENCE. 00021C UNTERVAL RESPECTIVELY. 00022C TL,TRLEFT- AND RIGHT-ENDPOINTS OF THE 00022C OUTPUT PARAMETERS: 00022C OUTPUT PARAMETERS: 00022C OUTPUT PARAMETERS: 00022C ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD TO CONVERGE. 00022C ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S 00030C METHOD TO CONVERGE. 00023C IFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING 00033 (D) FORMAT(' ITERATION NUMBER OF ITERATES 00034 THE L1 NORMS OF THE ITERATES 00035C COMPARISON OF THE ITERATES 00035C THE L1 NORMS OF THE ITERATES 00036 THE L1 NORMS OF THE ITERATES 00037 (D) FORMAT(' ITERATION NUMBER AND RESIDUAL:',/ 00038 C ' QUADRATIC CONVERGENCE IS EXPECTED.',/) 0037 D0 FORMAT(' ITERATION NUMBER AND RESIDUAL:',/ 00038 C ' QUADRATIC CONVERGENCE IS EXPECTED.',/) 0039 D0 350 LJ=1,ITMAX 00042C THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN 00042C THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN 00042C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) CONTAIN 00042C THE SUMMETRY OF (J). HENCE (SUB) AND (SUP) CONTAIN 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) CONTAIN 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 0004	00002C	
<pre>0004 INTEGER N,ITMAX,K,J,LJ,L,IFLAG 0005 REAL A(N),X(N),FX(50),AL,XL,AR,XR,DT,DA,T,W 0006 REAL SU(50),JD(6(50),SU(50),H(50),SUM1,SUM2 0007 REAL RATIO,GLEFT,GRIGH,EPS,FNORM1,TL,TR 00008 COMMON D(50),JD(50) 00009C 00010C INPUT PARAMETERS: 00011C 000112 AINITIAL ESTIMATE FOR NEWTON'S METHOD. 000132 00014C XKNOT SEQUENCE WITH THE ENDPOINTS DELETED. 00015C 00014C NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS. 00017C 00018C ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD. 00019C 00019C EPSPARAMETER USED TO TEST FOR CONVERGENCE. 00021C INTERVAL RESPECTIVELY. 00022C UL,TRLEFT- AND RIGHT-ENDPOINTS OF THE 00022C UTPUT PARAMETERS: 00022C OUTPUT PARAMETERS: 00022C OUTPUT PARAMETERS: 00022C ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD TO CONVERGE. 00027C ATHE CALCULATED ZERO IF CONVERGENCE OCCURRED. 00028C OUTPUT PARAMETERS: 00026C ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD TO CONVERGE. 00027C ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD TO CONVERGE. 00031C IFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING 00033C IFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING 00034C IFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX. 00035C 'QUADRATIC CONVERGENCE IS EXPECTED.',/) 00037 100 FORMAT(' ITERATION NUMBER AND RESIDUAL:',/ 00033 C 'QUADRATIC CONVERGENCE IS EXPECTED.',/) 00350 LJ=1,ITMAX 00040C THE ARRAYS (SUB), (DIAB), AND (SUP) CONTAIN 00041C THE ARRAYS (SUB), (DIAB), AND (SUP) CONTAIN 00042C THE ELMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE 00043C JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A). 00041C THE ARRAYS (SUB), (DIAB), AND (SUP) CONTAIN 00042C THE ELMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE 00043C JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A). 00044C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00045C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00045C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00045C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00045C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00045C THE SYMMETRY OF (J).</pre>	000030	
00005REAL A(N),X(N),FX(50),AL,XL,AR,XR,DT,DA,T,W00006REAL SUB(50),DIAG(50),SUP(50),H(50),SUM1,SUM200007REAL RATIO,GLEFT,GRIGH,EFS,FNORM1,TL,TR00008COMMON B(50),ID(50)000090000090000100INPUT PARAMETERS:000110AINITIAL ESTIMATE FOR NEWTON'S METHOD.000130000140000141XKNOT SEQUENCE WITH THE ENDPOINTS DELETED.000152NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.000170ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.000180ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.000190EPSPARAMETER USED TO TEST FOR CONVERGENCE.000210INTERVAL RESPECTIVELY.000220IT,TRLEFT- AND RIGHT-ENDPOINTS OF THE000231INTERVAL RESPECTIVELY.000220OUTPUT PARAMETERS:000220OUTPUT PARAMETERS:000220ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S000220ITHAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S000220ITHAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S000310IFLAG= 1: CONVERGENCE INDICATED BY COMPARING000320IFLAG= 2: NUMBER AND RESIDUAL:',/000331IFLAG= 2: NUMBER AND RESIDUAL:',/000340IFLAG= 2: NUMBER AND RESIDUAL:',/000350OUADATIC CONVERGENCE IS EXPECTED.',/)00350D 350 LJ=1,ITMAX000360FRINT 100000371OU FORMATC' ITERATION NUMBER AND RESIDUAL:',/000380C000390THE LEMENTS OF THE TRIDIAGONAL POSI	00004	INTEGER N, ITMAX, K, J, LJ, L, IFLAG
00006       REAL SUB(S0), DIAG(S0), SUP(S0), H(S0), SUM1, SUM2         00007       REAL RATIO, GLEFT, GRIGH, EPS, FNORM1, TL, TR         00008       COMMON D(S0), ID(S0)         000110       INPUT PARAMETERS:         000120       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         0001210       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         0001211       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         000132       AINTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.         000140       NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.         000170       ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.         000200       EPSPARAMETER USED TO TEST FOR CONVERGENCE.         000210       OUTPUT PARAMETERS:         000220       CUTPUT PARAMETERS:         000220       OUTPUT PARAMETERS:         000220       OUTPUT PARAMETERS:         000220       OUTPUT PARAMETERS:         000221       OUTPUT PARAMETERS:         000222       OUTPUT PARAMETERS:         000232       OUTPUT PARAMETERS:         000232       IFLAGIFLAGE 1: CONVERGENCE INDICATED BY COMPARING         000332       IFLAGIFLAGE 1: CONVERGENCE INDICATED BY COMPARING         000332       IFLAGIFLAGE 1: CONVERGENCE INDICATED BY COMPARING	00005	REAL A(N),X(N),FX(50),AL,XL,AR,XR,DT,DA,T,W
00007       REAL RATID.GLEFT.GRIGH.EPS,FNORM1,TL,TR         00008       COMMON D(50),ID(50)         00010C       INPUT PARAMETERS:         00011C       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         00012C       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         00013C       XKNOT SEQUENCE WITH THE ENDPOINTS DELETED.         00014C       XKNOT SEQUENCE WITH THE ENDPOINTS DELETED.         00015C       NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.         00017C       00018C         00018C       ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.         00019C       EPSPARAMETER USED TO TEST FOR CONVERGENCE.         00021C       OUPLOT PARAMETERS:         00022C       TL,TRLEFT- AND RIGHT-ENDPOINTS OF THE         00022C       OUTPUT PARAMETERS:         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD'S         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHON'S         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHON'S         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S <td>00006</td> <td>REAL SUB(50), DIAG(50), SUP(50), H(50), SUM1, SUM2</td>	00006	REAL SUB(50), DIAG(50), SUP(50), H(50), SUM1, SUM2
00008       COMMON D(50),ID(50)         00007C       INPUT PARAMETERS:         00011C       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         00012C       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         00013C       COMMON D(50),ID(50)         00014C       XKNDT SEQUENCE WITH THE ENDPOINTS DELETED.         00015C       NO014C         00014C       NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.         00017C       ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.         00018C       ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.         00020C       EPSPARAMETER USED TO TEST FOR CONVERGENCE.         00021C       INTERVAL RESPECTIVELY.         00022C       TL,TRLEFT- AND RIGHT-ENDPOINTS OF THE         00022C       OUTPUT PARAMETERS:         00022C       OUTPUT PARAMETERS:         00022C       OUTPUT PARAMETERS:         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S         00022C       ITHACNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S         00031C       ITELAGGIFLAGE 1: CONVERGENC	00007	REAL RATIO, GLEFT, GRIGH, EPS, FNORM1, TL, TR
00009C       INPUT PARAMETERS:         00011C       INPUT PARAMETERS:         00011C       AINITIAL ESTIMATE FOR NEWTON'S METHOD.         00013C       With the endpoints deleted.         00014C       XKNOT SEQUENCE WITH THE ENDPOINTS DELETED.         00015C       NTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.         00017C       With the second of the array (A): THE NUMBER OF UNKNOWNS.         00017C       ITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.         00017C       UO020C         00021C       LT,TRLEFT- AND RIGHT-ENDPOINTS OF THE         00022C       ILTREVAL RESPECTIVELY.         00022C       OUTPUT PARAMETERS:         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD'S         00022C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S         00032C       ITHEAS: NO	00008	COMMON D(50), ID(50)
00010CINPUT PARAMETERS:00011CAINITIAL ESTIMATE FOR NEWTON'S METHOD.00013CXKNDT SEQUENCE WITH THE ENDPOINTS DELETED.00014CXKNDT SEQUENCE WITH THE ENDPOINTS DELETED.00015CNTHE SIZE OF THE ARRAY (A): THE NUMBER OF UNKNOWNS.00017CITMAXMAXIMUM NUMBER OF ITERATIONS FOR NEWTON'S METHOD.00020CEPSPARAMETER USED TO TEST FOR CONVERGENCE.00021C00022C00022CTL,TRLEFT- AND RIGHT-ENDPOINTS OF THE00023CINTERVAL RESPECTIVELY.00024C00027C00024COUTPUT PARAMETERS:00025COUTPUT PARAMETERS:00026CMETHOD TO CONVERGENCE OCCURRED.00027CATHE CALCULATED ZERO IF CONVERGENCE OCCURRED.00028CITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S00030CMETHOD TO CONVERGE.0031CIFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING0033CIFLAGIFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.00033CIFLAGIFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.00033COO33C0033CYOU FORMAT(' ITERATION NUMBER AND RESIDUAL:',/00336C00337100 STO LJ=1,ITMAX0040700350 LJ=1,ITMAX00404CTHE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN0044CTHE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN0044CTHE ELEMENTS OF THE TRIDIAGONAL POSITUPE-DEFINITE0044CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE0044CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE0044CT	00009C	· · · · · · · · · · · · · · · · · · ·
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00021C       TL.TRLEFT- AND RIGHT-ENDPOINTS OF THE         00023C       INTERVAL RESPECTIVELY.         00024C       00025C         00025C       OUTPUT PARAMETERS:         00026C       00027C         00027C       ATHE CALCULATED ZERO IF CONVERGENCE DECURRED.         00028C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S         00030C       METHOD TO CONVERGE.         00031C       00032C         00032C       IFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING         00033C       THE L1 NORMS OF THE ITERATIONS EXCEEDED ITMAX.         00033C       IFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.         00033C       IFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.         00035C       00037 100         00037 100       FORMAT(' ITERATION NUMBER AND RESIDUAL:',/         00038       C       ' QUADRATIC CONVERGENCE IS EXPECTED.',/)         00039       D0 350 LJ=1,ITMAX         000400       THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN         00042C       THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE         0043C       JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).         0044C       IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,         0044C       IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,	000200	EPSPARAMETER USED TO TEST FOR CONVERGENCE.
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00024C       00027C       ATHE CALCULATED ZERO IF CONVERGENCE DECURRED.         00028C       00029C       ITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S         00030C       METHOD TO CONVERGE.         00031C       00032C       IFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING         00032C       IFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING         00033C       THE L1 NORMS OF THE ITERATES         00034C       IFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.         00035C       00037         00036       PRINT 100         00037       FORMAT(' ITERATION NUMBER AND RESIDUAL:',/         00038       C       ' QUADRATIC CONVERGENCE IS EXPECTED.',/)         00039       D0 350 LJ=1,ITMAX         000400       THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN         000402       THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN         000403       JACDBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).         0004402       THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE         0004402       THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF         0004403       JACDBIAN MATRIX (J), HENCE (SUB) AND (SUP) ARE         0004404       IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,         000450       THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE         000450 </td <td>000250</td> <td>OUTPUT PARAMETERS:</td>	000250	OUTPUT PARAMETERS:
00027CATHE CALCULATED ZERO IF CONVERGENCE OCCURRED.00028CITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S00030CMETHOD TO CONVERGE.00031CIFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING00032CIFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING00033CIFLAG= 2: NUMBER OF THE ITERATIONS EXCEEDED ITMAX.00035C0003600037100FORMAT(' ITERATION NUMBER AND RESIDUAL:',/00038C00039D0 350 LJ=1,ITMAX000400000410000410THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN000420THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE000431JACDBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).000440IT SHOULD BE NOTED. THAT THE MATRIX EQUATION SOLVER,000450THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF000460THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE000470BOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS000480FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.000490IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	000260	
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00029CITMAXNUMBER OF ITERATIONS REQUIRED FOR NEWTON'S METHOD TO CONVERGE.00031CMETHOD TO CONVERGE.00032CIFLAGIFLAG= 1: CONVERGENCE INDICATED BY COMPARING 00033C00032CIFLAGIFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.00034CIFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.00035CFORMAT(' ITERATION NUMBER AND RESIDUAL:',/00036FRINT 10000037 100FORMAT(' ITERATION NUMBER AND RESIDUAL:',/00038C' QUADRATIC CONVERGENCE IS EXFECTED.',/)00039D0 350 LJ=1,ITMAX00040CTHE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN00042CTHE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE00043CJACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00044CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00044CTHE SUBMERY OF (J). HENCE (SUB) AND (SUP)	00028C	
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00034CIFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.00035C00036PRINT 10000037 100FORMAT(' ITERATION NUMBER AND RESIDUAL:',/00038C' QUADRATIC CONVERGENCE IS EXPECTED.',/)00039D0 350 LJ=1,ITMAX00040CTHE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN00042CTHE ARRAYS OF THE TRIDIAGONAL POSITIVE-DEFINITE00043CJACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00045CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00046CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE00047CBOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.00049CIF D(K)=0.0 FOR SOME K. THEN THE NUMBER	000330	THE L1 NORMS OF THE ITERATES
00035C 00036 FRINT 100 00037 100 FORMAT(' ITERATION NUMBER AND RESIDUAL:',/ 00038 C ' QUADRATIC CONVERGENCE IS EXFECTED.',/) 00039 D0 350 LJ=1,ITMAX 00040C 00041C THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN 00042C THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE 00043C JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A). 00044C IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER, 00045C THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF 00046C THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE 00047C BDTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS 00048C FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL. 00049C IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00034C	IFLAG= 2: NUMBER OF ITERATIONS EXCEEDED ITMAX.
00036PRINT 10000037 100FORMAT(' ITERATION NUMBER AND RESIDUAL:',/00038C' QUADRATIC CONVERGENCE IS EXPECTED.',/)00039D0 350 LJ=1,ITMAX000400D0 350 LJ=1,ITMAX000410THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN000420THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE000430JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).000440IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,000450THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF000460THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE000470BOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS000480FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.000490IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	000350	
00037 100FORMAT(' ITERATION NUMBER AND RESIDUAL:',/00038C' QUADRATIC CONVERGENCE IS EXPECTED.',/)00039D0 350 LJ=1,ITMAX000400THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN000410THE ARRAYS OF THE TRIDIAGONAL POSITIVE-DEFINITE000420JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).000430JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).000440IT SHOULD BE NOTED. THAT THE MATRIX EQUATION SOLVER,000450THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF000460THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE000470BOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS000480FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.000490IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00036	PRINT 100
00038C' QUADRATIC CONVERGENCE IS EXPECTED.',/)00039D0 350 LJ=1,ITMAX00040CD0 350 LJ=1,ITMAX00041CTHE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN00042CTHE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE00043CJACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00045CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00046CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE00047CBOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.00049CIF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00037 100	FORMAT(' ITERATION NUMBER AND RESIDUAL: './
00039D0 350 LJ=1,ITMAX000400THE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN000410THE ARRAYS OF THE TRIDIAGONAL POSITIVE-DEFINITE000420THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE000430JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).000440IT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,000450THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF000460THE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE000470BOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS000480FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.000490IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00038 C	( PHATRATIC CONVERGENCE IS EXFECTED. (./)
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00041CTHE ARRAYS (SUB), (DIAG), AND (SUP) CONTAIN00042CTHE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE00043CJACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00045CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00046CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE00047CBDTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.00049CIF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00040C	
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00043CJACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00045CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00046CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE00047CBOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ABRAYS ARE WRITTEN OUT IN FULL.00049CIF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00042C	THE ELEMENTS OF THE TRIDIAGONAL POSITIVE-DEFINITE
00044CIT SHOULD BE NOTED.THAT THE MATRIX EQUATION SOLVER,00045CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00046CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE00047CBDTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ABRAYS ARE WRITTEN OUT IN FULL.00049CIF B(K)=0.0 FOR SOME K. THEN THE NUMBER	000430	JACOBIAN MATRIX (J), EVALUATED AT THE VECTOR (A).
00045CTHE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF00046CTHE SYMMETRY OF (J). HENCE (SUB) AND (SUP) ARE00047CBOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.00049CIF D(K)=0.0 FOR SOME K. THEN THE NUMBER	00044C	IT SHOULD BE NOTED. THAT THE MATRIX EQUATION SOLVER.
00046CTHE SYMMETRY OF (J), HENCE (SUB) AND (SUP) ARE00047CBOTH NECESSARY, ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.00049CIF D(K)=0.0 FOR SOME K. THEN THE NUMBER	00045C	THE SUBROUTINE (TRID), DOES NOT TAKE ADVANTAGE OF
00047CBOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1), EQUATIONS00048CFOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.00049CIF D(K)=0.0 FOR SOME K. THEN THE NUMBER	00046C	THE SYMMETRY OF (J), HENCE (SUB) AND (SUP) ARE
00048C FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL. 00049C 00050C IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	000470	BOTH NECESSARY. ALTHOUGH SUB(K)=SUP(K-1). EQUATIONS
00049C 00050C IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00048C	FOR BOTH ARRAYS ARE WRITTEN OUT IN FULL.
00050C IF B(K)=0.0 FOR SOME K. THEN THE NUMBER	00049C	
	000500	IF B(K)=0.0 FOR SOME K, THEN THE NUMBER

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000510	OF UNKNOWNS (AND EQUATIONS) REDUCE. IN ORDER
000520	TO PERMIT THE COMPUTATION OF ONE JACOBIAN
000530	MATRIX THE PROGRAM SETS SUB(K)=SUP(K-1)=0.0
00054C	AND DIAG(K)=1.0.
00 <b>055C</b>	
00056	DO 125 K=1.N
00057C	
00058	IF (K.EQ.1) THEN
00059	AI = 0.0
00060	XI = TI
00061	FISE
00062	AI = A(K-1)
00063	XI = X(K-1)
00064	END TE
000450	
000440	
000000	TE /K EO NN TUEN
00087	
00068	
00069	
00070	ELSE
00071	AK= A(K+1)
00072	XR = X(K+1)
00073	END IF
00074C	
00075C	
00076	IF ( AL.GE.0.0 .AND. A(K).GE.0.0 ) J1= 1
00077	IF ( AL.LT.0.0 .AND. A(K).GE.0.0 ) J1= 2
00078	IF ( AL.GE.O.O .AND. A(K).LT.O.O ) J1= 3
00079	IF ( AL.LE.0.0 .AND. A(K).LE.0.0 ) J1= 4
000800	
00081	IF ( A(K).GE.0.0 .AND. AR.GE.0.0 ) J2= 1
00082	IF ( A(K).LT.0.0 .AND. AR.GE.0.0 ) J2= 2
00083	IF ( A(K).GE.0.0 .AND. AR.LT.0.0 ) J2= 3
00084	IF ( A(K).LE.0.0 .AND. AR.LE.0.0 ) J2= 4
00085C	
00083	DT = X(K) - XL
00087	DA= A(K)-AL
00088C	
00089	IF ( ID(K) .EQ. 1) THEN
-00090C	
00091	IF (K.NE.1) THEN
000920	
00093	IF (.11.FQ.1) THEN
000940	
00095	$SUB(K) = TIT/A_0$
00073	B EET = DT/3.0
00070	04417- 1170+V
00000	
00078	EFOE IL (DI*EK+5) HEM
00100	T = YI = (T)T (T)A YA
00101	17 ALTAU/UN/ANL N- A FW/ Y/KAITA
AATAT	₩~ ♡+3みく 入(八ノキ) ノ

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00124C 00125 00126 00152 00148 00136 00137C 00127 00111 00112 00113 00113 00114 00151 00150 00149 00143 00142 001350 00131 00132C 001300 00120C 00121 00122C 00119 00104 00105 00106C 00107 00147 00145 00141C 00140 00138 00134 00133 00129 00123 00118 00109 00146C 00144C 001390 001280 00115 00110 00102 00117C 001080 n c n  $\mathbf{O}$ C)  $\mathbf{c}$ T= XL-(DT/DA)\* W= 0.5\*(T+XL SUB(K)= (T-XL) SUB(K)= GLEFT= Ê SUB(K)= GLEFT= I GLEFT= IF (J1 **ELSE** GLEFT= SUB(K) =닡 ELSE IF ( ID(K) SUR(1) =GLEFT= SUB(K)='0+0 GLEFT= GLEFT= SUB(K) == XL-(DT/DA)\*AL = 0.5\*( X(K)+T ) UB(K)= (X(K)-T)/6.0 % EFT= 0.0 (J1.EQ.1) XL-(IT/IA)\*AL 닊 ELSE END IF 믂 = DT/6.0 DT/3.0 (K.NE.1) DT/6.0 DT/3.0 0.0 0.0 (T-XL)/6.0 ELSE IF ( ID(K) ENI ELSE (X(K)-T)/6.0 \* ( ((T-XL)/DT)\*((X(K)-T)/DT) + 4.0\*((U-XL)/DT)\*((X(K)-U)/DT) ) IF (J1.EQ.4) (T-XL)/6+0 \* ( 4+0\*(((W-XL)/DT)\*\*2) + ((T-XL)/DT)\*\*2 ) 片 ELSE IF (J1.EQ.3) THEN (X(K)-T)/6+0 \* ( ((T-XL)/DT)\*\*2 + 4+0\*(((W-XL)/DT)\*\*2) + 1 닊 (K.EQ.1) + GLEFT= ¦ .)/6+0 \* ( 4+0\*((W-XL)/DT)\*((X(K)-W)/DT) + ((T-XL)/DT)\*((X(K)-T)/DT) )  $\sim$ 4.0\*(((W-XL)/DT)\*\*2) + 1.0 ) THEN ·EQ. (J1.E0.3) . (J1.EQ.4) THEN н О DT/3.0 THEN 0 THEN - $\sim$  $\sim$ THEN THEN THEN 1.0 >

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00191C 00192 00193C 00180 00181 00182 00183 00199 00197 00190 001890 00188 00186C 00187 00185 00184 00173 00174 00175C 00167C 00168 00169C 00202 00196 00194 00195C 00178 00176 00177C 00203 00201 00172 00171C 00170 00165 00162C 00163 00161 00158 00159 00155C 00156 00157 00153C 00154 002000 001980 00166 00160 001790 00164C  $\mathbf{c}$  $\mathbf{n}$ T= X(K)-W= 0.5\*( SUP(K)= SUP(K)= GRIGH= IIA= IIT= END GLEFT= IF (J1 SUB(K)= GLEFT= END 片 片片 SUB(1) =Ē GLEFT= SUB(K)= 님 X(K)-(DT/DA)\*A(K) 0.5\*( XR+T ) (K•NE•1) ( D(K-1)  $\sim$ (J1.EQ.4) 0.5\*( XL-(DT 爿뉘 벆 AR-A(K) END XR-X(K) ELSE 닊 SUB(K) GLEFT ID(K+1) (K.NE.N) IIT/6.0 0.0 닊 0.0 0.0 (T-XL)/6.0 (XR-T)/6.0 ELSE DT/3.0 묶 END **ELSE** ELSE (T-XL)/6. 片 T+XL /IIA) \*AL (J2.EQ.1) .EQ. 11 11 뷰 (K.EQ.1) 닊 GLEFT= •EQ. 片 00.0 닊 + +  $\sim$ ((T-XL)/DT)\*\*2 ((T-XL)/DT)\*((X(K)-T)/DT) ) 6+0 \* ( 4+0\*((U-XL)/DT)\*\*2) THEN (J2.E0.2) (J1.EQ.2) (J1.EQ.1) THEN 0,0 **---**÷e × IIT/3.0 - $\sim$ THEN THEN J ~ THEN THEN 4.0\*((W-XL)/DT)\*((X(K)-W)/DT) ((T-X(K))/DT)\*((XR-T)/DT) THEN THEN J ٠

00204 C + 4.0\*((W-X(K))/DT)\*((XR-W)/DT) ) 00205 GRIGH= (XR-T)/6+0 \* ( ((XR-T)/DT)\*\*2 00206 С + 4.0\*(((XR-W)/DT)\*\*2) ) 002070 00208 ELSE IF (J2.E0.3) THEN 002090 00210 T = X(K) - (DT/DA) \* A(K)W = 0.5\*(T+X(K))00211 00212 SUP(K)= (T-X(K))/6.0 \* ( 4.0\*((W-X(K))/DT)\*((XR-W)/DT) С 00213 + ((T-X(K))/DT)\*((XR-T)/DT) ) 00214 GRIGH= (T-X(K))/6.0 \* ( 1.0 + 4.0\*(((XR-W)/DT)\*\*2) 00215 3 + ((XR-T)/DT)\*\*2 ) 00213C ELSE IF (J2.EQ.4) THEN 00217 00218C 00219 SUP(K) = 0.000220 GRIGH= 0.0 002210 00222 END IF 00223C 00224 ELSE IF (K.EQ.N) THEN 00225C 00226 SUP(N) = 0.000227 GRIGH= 0.0 00228 IF (J2.EQ.1) GRIGH= DT/3.0 002290 00230 END IF 00231C ELSE IF ( ID(K+1) .EQ. 0 ) THEN 00232 00233C 00234 SUP(K) = DT/6.0GRIGH= DT/3.0 00235 00236C 00237 ELSE IF ( ID(K+1) .EQ. -1 ) THEN 00238C 00239 IF (K.NE.N) THEN 00240C 00241 IF (J2.EQ.4) THEN 00242C 00243 SUP(K) = IIT/6.000244 GRIGH= DT/3.0 00245C ELSE IF (J2.EQ.3) THEN 00246 002470 00248 T = X(K) - (DT/DA) \* A(K)00249 W = 0.5\*(XR+T)00250 SUP(K)= (XR-T)/6.0 \* ( ((T-X(K))/DT)\*((XR-T)/DT) 00251 С + 4.0\*((W-X(K))/DT)\*((XR-W)/DT) ) 00252 (XR-T)/6.0 \* ( ((XR-T)/DT)\*\*2 GRIGH= С 00253 + 4.0\*(((XR-W)/DT)\*\*2) ) 00254C

00255 ELSE IF (J2.E0.2) THEN 002560 00257 T = X(K) - (DT/DA) \* A(K)00258 W = 0.5 \* (T + X(K))00259 SUP(K) = (T-X(K))/6.0 \* (4.0\*((W-X(K))/DT)\*((XR-W)/DT))+ ((T-X(K))/DT)\*((XR-T)/DT) ) 00260 С 00261 (T-X(K))/6.0 \* ( 1.0 + 4.0\*(((XR-W)/DT)\*\*2) GRIGH= С 00262 + ((XR-T)/DT)\*\*2 ) 002630 00264 ELSE IF (J2.E0.1) THEN 00265C 00266 SUP(K) = 0.000267 GRIGH= 0.0 00268C 00269 END IF 00270C ELSE IF (K.EQ.N) THEN 00271 00272C 00273 SUP(N) = 0.000274 GRIGH= 0.0 00275 IF (J2.EQ.4) GRIGH= DT/3.0 00276C 00277 END IF 00278C 00279 END IF 00280C 00281 IF (K.NE.N) THEN 00282 IF ( D(K+1) .EQ. 0.0 ) THEN 00283 SUP(K) = 0.000284 GRIGH = 0.0END IF 00285 END IF 00286 002870 00288 DIAG(K) = GLEFT+GRIGH 002890 00290C 00291 IF ( D(K) .EQ. 0.0 ) THEN 00292 DIAG(K) = 1.000293 SUB(K) =0.0 00294 SUP(K)= 0.0 00295 END IF 00296C 00297 125 CONTINUE 002980 00299 DO 150 L=1.N 00300 H(L) = D(L)00301 150 CONTINUE 003020 003030 00304C WE SOLVE THE MATRIX EQUATION JX=H, THE ARRAY (H)

00305C BEING IDENTICAL TO THE ARRAY (D). THE SOLUTION 00304C IS RETURNED IN THE ARRAY (H). 00307C 00308C 00309 CALL TRID(SUB, DIAG, SUF, H, N) 003100 00311 SUM1= 0.0 DO 200 L=1,N 00312 00313 A(L) = H(L)SUM1= SUM1 + ABS(A(L)) 00314 00315 200 CONTINUE 00316C 00317C THE FUNCTION EVALUATION SUBROUTINE COMPUT MAY 00318C BE DELETED. IN THIS CASE THE FOLLOWING EIGHT LINES ARE TO BE DELETED AND THE ARRAY (FX) 003190 00320C CAN BE TAKEN FROM THE REAL STATEMENT AT THE 003210 BEGINNING OF THIS SUBROUTINE. 00322C 00323 CALL COMPUT(A,FX,N,X,TL,TR) 00324 FNORM1= 0.0 00325 DO 250 L=1,N . FNORM1 = FNORM1 + FX(L)\*FX(L) 00326 00327 250 CONTINUE 00328 FNORM1= SQRT(FNORM1) 00329 WRITE(6,300) LJ,FNORM1 00330 300 FORMAT(15,E15.6) 003310 003320 00333 IF (LJ.NE.1) THEN 00334 RATID= ABS(SUM1-SUM2) 00335 AB= EPS\*SUM2 IFLAG= 1 00336 00337 IF (RATIO .LE. AB) GO TO 400 END IF 00338 00339 SUM2= SUM1 00340 350 CONTINUE 00341 IFLAG= 2 00342 400 CONTINUE 00343 ITMAX= LJ 00344 RETURN 00345 END

00001	SUBROUTINE COMPUT(A,FX,N,X,TL,TR)
000020	
000030	SUBROUTINE (COMPUT), THE FUNCTION EVAULATING
00004C	SUBROUTINE, IS OFTIONAL.
000050	
00006C	
00007	REAL A(N).FX(N).F1.ALD.AHI.TLD.THT
00008	REAL GLEF-GRIG-TS-X(N)
00009	INTEGER N.K. II. 12
00010	COMMON T(50) TT(50)
00011	$T_{10} = 100 \text{ K} = 1.8$
000120	
00013	
000140	
00015	TE (KAERAI) THEN
00016	Al D = 0.0
00017	
00019	
00010	$AL \Omega = A(K-1)$
00020	$\frac{1}{10} = \frac{1}{10} \frac{1}{10}$
00021	FND TE
000220	
000220	TE (K.ED.N) THEN
00024	AHI = 0.0
00025	
00026	FISE
00020	ΔUT- Δ(K11)
00029	
00020	
00029	CHD TL
000310	
000010	
000320	TE (ALC GE O O AND A(K) GE O O) 11-1
00033	TE (ALB, IT, 0, 0 AND A(K), GE 0, 0) II = 7
00035	TE (A   B   EE   A   A   A   A   A   A   A   A
00034	IF $(A   D,   T, 0, 0, AND, A(K),   T, 0, 0)   1 = 4$
000370	
00038	IE (A(K), GE(0, 0), ANT, AHT, GE(0, 0), I2= 1
00039	IF $(A(K), I, T, 0, 0)$ AND, AHI, GE, 0, 0) $I2= 2$
00040	TF (A(K), GF, 0, 0) AND, AHT, (T, 0, 0) 12= 3
00041	IF (A(K), I, T, O, O, AND, AHI, I, T, O, O) = A
000420	1 (N(K/) E1+0+0 (IN(E+ )))1+E1+0+0/ 520 4
000420	
000440	DI - MINZ FLU
00045	TE ( TD(K) .ED. 1 ) THEN
000460	TI V TRAINA + FREAT A TURENA
00047	TE ( 11 EO 1) TUEN
00042	TE VATAERATI LUEN
000400	GLEE = DTx(2, DxA(K) + ALD )/ALD
000500	www. Alter Levening, I HEW // Utv
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66000 00097 000960 00092C 00093 00094C 00089 00087 00083C 00084 00085C 98000 00077C 00072 00073C 00071C 00101 56000 00091 00078 00074 00069C 89000 00065C 000980 00082 00081 00076 00066 00062 000610 00053 00051 00052C 001000 000880 00080 000790 000750 00070 00064 00060 00059 00057 00055 00067C 000630 000580 000560 L TS= TI F1= ( GLEF= <u>=</u>= GLEF= GLEF= TS= GLEF= TS= TI GLEF= TS= GLEF= GLEF= GLEF= END 110 EL SE TLO THI-X(K) ELSE 埍 ~ 10 0.0 IIT\*( DT\*( \_D - ALD\*DT/( A(K)-ALD ) (TS+X(K))\*0.5 - TLO )/DT (X(K)-TS)\*A(K)\*( 2.0\*F1 (X(K)-TS)\*A(K)\*( 0 - ALO\*DT/( A(K)-ALO (TS+X(K))\*0.5 - TLO ), 0 ~ ~ õ Ę END ELSE - ALD\*DT/( A(K)-ALD ) (TS-TLD)\*\*2 )\*ALD/(6+0\*DT) ELSE 믂 ENI ELSE 믂 ELSE - ALD\*DT/( A(K)-ALD ) (TS-TLD)\*\*2 )\*ALD/(6.0\*DT) ELSE ELSE IF 붂 ID(K+1) (J2.EQ.1) 2.0\*A(K) (J1.EQ.4) 2.0\*A(K) 닊 ~  $\sim$ H IF F 묶 F Ħ 닊 ID(K) II(K) (J1.EQ.3) (J1.EQ.2) (J1.EQ.1) THEN (J1.EQ.4) THEN (J1.EQ.3) (J1.EQ.2) •EQ• + •EQ• +-•EQ• THEN THEN **....** TLO )/DT ALO AL O 2.0\*F1  $\cup$ 0 1 THEN THEN THEN THEN THEN )/6.0 يت ا >/6.0 J **\_**  $\sim$ THEN + THEN + ه. 1.0 0 )/6.0 )/6.0

00102C 00103 GRIG= DT\*( 2.0\*A(K) + AHI )/6.0 00104C 00105 ELSE IF (J2.EQ.2) THEN 00106C 00107 TS = X(K) - A(K) \* DT/(AHI - A(K))00108 GRIG= ( (THI-TS)\*\*2 )\*AHI/(6.0\*DT) 001090 ELSE IF (J2.EQ.3) THEN 00110 001110 00112 TS = X(K) - A(K) \* DT/(AHI - A(K))00113 F1= ( THI-0.5\*( TS+X(K) ) )/DT GRIG= ( TS-X(K) )\*A(K)\*( 1.0 + 2.0\*F1 )/6.0 00114 00115C 00116 ELSE IF (J2.EQ.4) THEN 00117C 00118 · GRIG= 0.0 ·00119C END IF 00120 00121C ELSE IF ( ID(K+1) .EQ. 0 ) THEN 00122 001230 00124 GRIG= DT\*( 2.0\*A(K) + AHI )/6.0 00125C 00126 ELSE IF ( ID(K+1) .EQ. -1 ) THEN 001270 00128 IF (J2.EQ.4) THEN 00129C GRIG= DT\*( 2.0\*A(K) + AHI )/6.0 00130 001310 00132 ELSE IF (J2.EQ.3) THEN 00133C TS = X(K) - A(K) \* DT/(AHI - A(K))00134 GRIG= ( (THI-TS)\*\*2 )\*AHI/(6.0\*DT) 00135 001360 ELSE IF (J2.EQ.2) THEN 00137 00138C TS= X(K) - A(K) \* DT/(AHI-A(K))00139 00140 F1= (THI-0.5\*(TS+X(K)))/DT00141 GRIG= ( TS-X(K) )\*A(K)\*( 1.0 + 2.0\*F1 )/6.0 00142C ELSE IF (J2.EQ.1) THEN 00143 00144C 00145 GRIG= 0.0 00146C 00147 END IF 00148C 00149 END IF 001500 001510 00152 IF (K.NE.1) THEN

IF ( D(K-1) .EQ. 0.0 ) GLEF= 0.0 00153 END IF 00154 . 00155C 00156 IF (K.NE.N) THEN 00157 IF ( D(K+1) .ER. 0.0 ) GRIG= 0.0 00158 END IF 001590 00160 FX(K) = GLEF + GRIG - D(K)00161C 00162 ELSE IF ( D(K) .EQ. 0.0 ) THEN 00163 FX(K) = 0.000164 END IF 001650 00166 100 CONTINUE RETURN 00167 00168 END

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00001	SUBROUTINE POLY(A,T;PP,M,F,LI,TX)
000020	
000030	SUBROUTINE POLY INTEGRATES BACK TWICE THE
00004C	POSITIVE PART OF THE PIECEWISE LINEAR SECOND
000050	DERIVATIVE WHERE THE DATA SUGGESTS THAT THE
00006C	INTERPOLATING CURVE SHOULD BE CONVEX, THE
00007C	NEGATIVE PART OF THE PIECEWISE LINEAR SECOND
000080	DERIVATIVE WHERE THE DATA SUGGESTS THAT THE
00009C	INTERPOLATING CURVE SHOULD BE CONCAVE, AND
000100	THE REMAINING PORTION OF THE PIECEWISE LINEAR
00011C	SECOND DERIVATIVE ON THE TRANSITION INTERVALS.
00012C	
000130	THE INTEGRATION YIELDS A PIECEWISE CUBIC
00014C	POLYNOMIAL WITH KNOTS GIVEN BY THE SEQUENCE
000150	(TX). THIS CUBIC POLYNOMIAL INTERPOLATES THE
000160	DATA AND ITS COEFFICIENTS ARE DENOTED BY THE
000170	NUMBERS PP(J,I) - THE VALUE OF THE (J-1)ST
000180	DERIVATIVE OF THE FUNCTION EVALUATED AT TX(I).
000190	FOR X SUCH THAT TX(I).GE.X.LT.TX(I+1) THE VALUE
000200	OF THE CUBIC POLYNOMIAL IS
000210	
000220	PP(1,I)
000230	+ PP(2,I) * ( X-TX(I) )
00024C	+ (1/2)PP(3,1) * ( X-TX(1) )**2
000250	+ (1/6)PP(4,I) * ( X-TX(I) )**3
000260	
00027C	
00028	INTEGER M, J, L, LI
00029	REAL A(50),T(50),PP(4,100),F(50),TX(100),TAU
00030	REAL DF, DT, DA, C, E
00031	COMMON D(50),ID(50)
00032	LI= 1
00033	MN1= H-1
00034	NO 100 L=1,MN1
00035	IF = F(L+1) - F(L)
00036	DT = T(L+1) - T(L)
00037	IA= A(L+1)-A(L)
000380	
00039	JP= 0
00040	IF (L.EQ.1) THEN
00041	IF ( D(1) .EQ. 0.0 ) JP= 1
00042	ELSE IF (L.EQ.MN1) THEN
00043	IF ( $D(M-2)$ , EQ. 0.0 ) $JP=1$
00044	ELSE
00045	C= D(L-1)*D(L)
00046	JF ( C .EQ. 0.0 ) JP= 1
00047	END IF
000480	
00049C	
000500	

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00073
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00063
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00067
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00052C
        00100
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                                                    000940
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                                                                                                                     PP(4,LI)=
PP(3,LI)=
PP(2,LI)=
                                                                                                                                                                                                            C= IF/11 -
PP(4,LI)=
PP(3,LI)=
              E= F(L) -
C= DF/DT +
                                                                                                                                                                                                                                                                                                                                                 PP(4,LI)=
PP(3,LI)=
PP(2,LI)=
                                                            TX(LI+1)=
LI= LI+2
      PP(4,LI) =
                              TAU=
                                                                                 PP(1,LI+1) =
                                                                                               PP(4,LI+1)= DA/DT
PP(3,LI+1)= 0.0
                                                                                                             PP(1,LI)=
                                                                                                                                            Ŷ
                                                                                                                                                   TAU=
                                                                                                                                                                                 FF(1,LI)=
                                                                                                                                                                                                      PP(2,LI)=
                                                                                                                                                                                                                                                                         ELSE
                                                                                                                                                                                                                                                                                                                                                                                묶
PP(3,LI) =
                                                                                         PP(2,LI+1)=
                                                                                                                                                                                                                                                                                                                             LI = LI+1
                                                                                                                                                                                                                                                                                                                                    PP(1,LI)= F(L)
TX(LI)= T(L)
                                                                          TX(LI) = T(L)
                                                                                                                                                                                         TX(LI) = T(L)
                                                                                                                                                                                                                                                                               (A(L).LT.0.0
(A(L).GT.0.0
                                                                                                                                            DF/DT
              DF/DT + (A(L)**3)*DT/(6.0*DA*DA)
                                                                                                                                                                                                                                                                         (A(L).LE.0.0
                                                                                                                                                                                                                                                                                               (A(L).GE.0.0
                                                                                                                                                                                                                                                                                                                                                                                (JP.EQ.1)
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                              T(L)
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                                                                   TAU
                                                                                                              F(L)
        IIA/IIT
A(L)
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                                                                                                                                                                                                                                                                                                                                                 0+0
0+0
IIF/IIT
                     (A(L)**3)*DT*DT/(6.0*DA*DA)
                                                                                                                            0.0
                                                                                                                                                                                                              A(L)
                               1
                                                                                                                      C
                                                                                                                                                                                                                       DA/DT
                                                                                                                                                                                                                                            (J.EQ.1)
                                                                                                                                            (A(L+1)**3)*DT/(6.0*DA*DA)
                                                                                                                                                                                                                             (IA/6.0
                                                                                  C*(TAU-T(L))
                                                                                                                                                   A(L)*DT/DA
                              A(L) XIIT/IIA
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                                             묶
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                                                                                                                                                                                                                                                                                        .AND.
                                                                                                                                                                                                                                                                         . AND.
                                                                                                                                                                                                                                                                                                .AND.
                                                                                                                                                                   (J.EQ.2)
                                                                                                                                                                                                                                                                                • AND •
                                             (J.EQ.3)
                                                                                                                                                                                                                                                                                                               THEN
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                                                                                                                                                                                                                                             THEN
                                                                                                                                                                                                                                                          C
                                                                                                                                                                                                                                                                               A(L+1).GE.0.0)
A(L+1).GT.0.0)
A(L+1).LT.0.0)
                                                                                                                                                                                                                             A(L)/2.0)*DT
                                                                                                                                                                                                                                                                         A(L+1).LE.0.0)
                                                                                                                                                                                                                                                          THEN
                                             THEN
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                                                                                                                                                                   THEN
                                                                                  F(L)
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00102 PP(2,LI) = C + A(L)\*A(L)\*DT\*0.5/DA00103 PP(1,LI) = F(L)00104 PP(4,LI+1) = 0.000105 FF(3,LI+1) = 0.000106 PP(2,LI+1) = C00107 PP(1,LI+1) = C\*(TAU-T(L)) + E00108 TX(LI) = T(L)00109 TX(LI+1) = TAU00110 LI = LI+2001110 00112 ELSE IF (J.EQ.4) THEN 001130 PP(4,LI) = 0.000114 PP(3,LI) = 0.000115 PP(2,LI)= DF/DT 00115 00117 PP(1,LI) = F(L)00118 TX(LI) = T(L)00119 LI = LI+1001200 00121 END IF 00122C 00123 ELSE IF ( III(L) .EQ. 0 ) THEN 00124C 00125 C = DF/DT - (DA/6.0 + A(L)/2.0) \*DT00126 PP(4,LI) = IIA/IITPP(3,LI) = A(L)00127 00128 PP(2,LI) = C00129 FF(1,LI) = F(L)00130 TX(LI) = T(L)00131 LI = LI + 100132C 00133 ELSE IF ( ID(L) .EQ. -1 ) THEN 00134C 00135 IF (J.EQ.4) THEN 00136C 00137 C= DF/DT - (DA/6.0 + A(L)/2.0)\*DT 00138 PP(4,LI) = IIA/IIT00139 PP(3,LI) = A(L)00140 PP(2,LI) = C00141 PP(1,LI) = F(L)00142 TX(LI) = T(L)00143 LI = LI + 100144C 00145 ELSE IF (J.EQ.3) THEN 00146C 00147 TAU= T(L) - A(L)\*DT/DA C= DF/DT - (A(L+1)\*\*3)\*DT/(6.0\*DA\*DA) 00148 00149 PP(4,LI)= 0.0 00150 PP(3,LI) = 0.000151 PP(2,LI) = C00152 PP(1,LI) = F(L)

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00153
             PP(4,LI+1) = DA/DT
00154
             PP(3,LI+1) = 0.0
00155
             PP(2,LI+1) = C
00156
             PP(1,LI+1) = C*(TAU-T(L)) + F(L)
00157
             TX(LI) = T(L)
00158
             TX(LI+1) = TAU
00159
             LI= LI+2
00160C
00161
                      ELSE IF (J.EQ.2) THEN
001620
00163
             TAU= T(L) - A(L) \times DT/DA
00164
             E = F(L) - (A(L)**3)*DT*DT/(6.0*DA*DA)
00165
             C= DF/DT + (A(L)**3)*DT/(6.0*DA*DA)
00166
             PP(4,LI)= DA/DT
00167
             PP(3,LI) = A(L)
00168
             PP(2,LI) = C + A(L)*A(L)*DT*0.5/DA
             PP(1,LI) = F(L)
00169
00170
             PP(4,LI+1) = 0.0
00171
             PP(3,LI+1) = 0.0
00172
            · PP(2,LI+1)= C
             PP(1,LI+1)= C*( TAU-T(L) ) + E
00173
00174
             TX(LI) = T(L)
00175
             TX(LI+1) = TAU
00176
             LI = LI + 2
00177C
00178
                      ELSE IF (J.EQ.1) THEN
001790
00180
             PP(4, LI) = 0.0
00181
             PP(3,LI) = 0.0
00182
             PP(2,LI)= DF/DT
00183
             PP(1,LI) = F(L)
             TX(LI) = T(L)
00184
00185
             LI = LI + 1
00186C
00187
                     END IF
00188C
00189
                 END IF
00190C
00191
             END IF
001920
00193 100
             CONTINUE
00194
             PP(4,LI) = 0.0
00195
             PP(3,LI) = 0.0
00196
             PP(2,LI) = 0.0
00197
             PP(1,LI) = F(M)
00198
             TX(LI) = T(M)
00199
             RETURN
00200
             END
```

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## Autobiographical Statement

The author was born in Ironton, Ohio on July 15, 1959. He received the Bachelor of Science degree in mathematics from Georgetown College in Georgetown, Kentucky in May 1981. He received the Master of Science degree in computational and applied mathematics from Old Dominion University in December 1982. As a doctoral candidate the author was supported by a fellowship by the Institute for Computational and Applied Mechanics. He is co-author along with Drs. Philip W. Smith and Samuel P. Marin of "Constrained Interpolation and Smoothing," General Motors Research Report Number MA-312.