ON THE NUMERICAL CONSTRUCTION AND APPROXIMATION OF SOME PIECEWISE POLYNOMIAL FUNCTIONS

by

D. S. Meek

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Abstract

For any odd order polynomial spline defined in terms of even derivatives on a uniformly spaced set of knots, a formulation of the defining equations is discussed for which the successive overrelaxation iterative method is proved to converge. Supporting numerical results are displayed.

The notion of multiple spline approximation is investigated for the cubic spline and once it has been established that there can be some advantage to using this process, further general forms of periodic multiple spline approximation on uniform partitions are examined. For completeness, the explicit formulae for the leading term of the truncation error of odd and even order polynomial splines, interpolating either at the knots or midway between the knots, are developed. An application of multiple cubic splines to the solution of a class of second order linear differential equations is compared with some common numerical procedures. Further applications of multiple splines to the estimation of various higher order derivatives of a tabulated periodic function are made and some useful error bounds obtained.

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Chapter 1

Introduction

1.1. Scope of thesis

Several problems are investigated in this thesis. The first is the numerical construction of odd degree polynomial splines defined in terms of their even derivatives. Another problem is that of approximating the derivative of a given function which is known only at a number of discrete points. The approximations so found are then used to solve a boundary value problem.

1.2. Numerical construction of polynomial splines

In numerical work, splines are commonly expressed in terms of their various derivatives at the knots. Ahlberg, Nilson and Walsh [4] set up the equations for both cubic splines and general odd-degree splines while Späth [41] has obtained a block upper Hessenberg form of equations for odd-degree splines. If the odd-degree splines are defined on a uniform partition, Albasiny and Hoskins [6] obtain a block upper Hessenberg form for the equations. A somewhat novel method of solving this latter set of equations (by reducing it first to block tridiagonal form) is developed and discussed in detail in Chapter 2.

Several authors have published algorithms in the form of computer programs to solve for the derivatives of cubic splines (Greville [19], Späth [40]).

Another method for obtaining a spline approximation (which is not used here) is to express the spline as a linear combination of basis splines. Both Schumaker [36] and Carasso and Laurent [13] recommend using B-splines as the basis splines and in both cases a band type of matrix is obtained. A convenient, numerically stable algorithm for evaluating B-splines is given by de Böor [12].

1.3. Error analysis of splines and multiple splines

The error in spline approximation may be expressed either as the L_∞ norm of the difference between the function being approximated and the spline, or as the L_2 norm of the Peano kernel of the spline operator (Secrest [37], Greville [19]).

Many authors have discussed the order of approximation of the cubic spline to a given function, including Ahlberg and Nilson [3], Birkhoff and de Boor [9], Sharma and Meir [38], Atkinson [8], and Sonneveld [39]. The orders of approximation of a spline function to a given function and its derivatives have been calculated for general odd-order splines by Ahlberg et al.[4], de Boor [10], and Swartz [43]. In Chapter 3, explicit bounds are obtained on the error in approximation of various cubic multiple splines to derivatives of a function whereas previously only numerical evidence [4] indicated the accuracy of multiple spline approximations. Several authors, [7] and [42], have given the leading term of the error in approximation of general odd-degree splines defined on a uniform partition to a function and its derivatives. Their results are extended in Chapter 4 to include both even and odd-degree splines defined both at the knots and at the midpoints of the intervals. Two general theorems on the infinity norms of certain types of matrices yield new bounds for the errors in approximation of periodic splines to periodic functions. Bounds on the error in approximation of various periodic multiple splines to derivatives of a periodic function are calculated explicitly in Chapter 5.

The use of multiple spline approximations to derivatives of a given function is motivated by the fact that high order polynomial spline approximation often tends to be too oscillatory. Multiple spline approximation to various derivatives of a function are generally more accurate than single spline approximation and are constructed using low order polynomials to avoid undesirable oscillations.

Chapter 2

Iterative Solution of Odd-Degree Polynomial Splines on a Uniform Partition

2.1 Defining equations of the $2r + 1$ st order spline

2.1.1 Introduction

This chapter is concerned with polynomial splines of order $2r + 1$ defined on the uniform partition Π : $x_j = x_0 + jh$, $j = 0,1,\ldots,n$ of the interval $[x_0, x_n]$. If $s(x)$ is the spline function and $y(x)$ is the function being approximated on the partition Π, then $s(x)$ satisfies the conditions:

(i) $s(x)$ is a polynomial of degree $2r + 1$ in $[x_j, x_{j+1}]$, $j = 0,1,\ldots,n-1$,

(ii) $s(x)$ interpolates to the values $y_j = y(x_j)$,

(iii) $s(x) \in C^{2r} [x_0, x_n]$.

In the literature odd-degree polynomial splines are usually discussed since proofs for their existence and uniqueness have been constructed for a variety of boundary conditions (Ahlberg et al. [4,p.109], Kershaw [29]). In not all of these cases do the corresponding even degree polynomial splines exist [4] ; moreover, the equations defining the general polynomial spline on a set of unequal intervals are generally too cumbersome to work with directly for any order greater than three, and recourse must be made to the forms of Cox [14] or de Boor [12]. The equations describing the spline of order $2r + 1$ are of a particularly simple form when the spline is defined on a uniform partition with linear boundary conditions, and in this case the describing equations form a set of simultaneous equations with a coefficient matrix of band form with band width $2r + 1$.

A formulation based on the even derivatives of the $2r + 1$ st order polynomial spline $s(x)$ defined on a non-uniform partition of $[x_0, x_n]$, has been given by Spath [41]. The boundary conditions $s^{(2k)}(x_0)$ and $s^{(2k)}(x_n)$, $k = 1,2,\ldots,r$ were in this case assumed known and resulted in the coefficient matrix of the defining equations being a block upper Hessenberg matrix with tridiagonal blocks. Solution of this set of equations was by successive under-relaxation (SUR) and the optimal SUR parameter , w_b , was found empirically.

A further formulation based on even derivatives was made by Albasiny and Hoskins [6] and once again a block upper Hessenberg matrix with tridiagonal blocks was obtained. Solution this time was by SOR and convergence for this form was faster than that quoted in [41].

In this chapter, the equations developed by Albasiny and Hoskins [6] are reordered in such a way that the optimal SOR parameter can be determined theoretically and the convergence of the SOR iterative method established for all odd-order splines.

2.1.2 Development of defining equations for the $2r + 1$ st order spline on a uniform partition

The development of the equations for the spline is essentially that of Albasiny and Hoskins [6] and is detailed here briefly for clarity of exposition.

In each interval of the partition Π the spline $s(x)$ is a polynomial of degree $2r + 1$ and therefore, assuming the even derivatives are continuous at each interior point x_j, $j = 1,2,\ldots,n-1$, the following finite Taylor series expansions hold

$$s_{j+1}^{(2r)} = s_j^{(2r)} + h s_{j_R}^{(2r+1)}$$

and

$$s_{j-1}^{(2r)} = s_j^{(2r)} - h s_{i_L}^{(2r+1)} ,$$

where R and L denote right and left limits respectively for the derivatives. Adding the two above equations produces

$$\delta^2 s_j^{(2r)} = h(s_{j_R}^{(2r+1)} - s_{j_L}^{(2r+1)}) . \qquad (2.1\text{-}1)$$

Use of finite Taylor series expansions gives the further equations

$$s_{j+1}^{(2r-2)} = s_j^{(2r-2)} + h\, s_{j_R}^{(2r-1)} + \frac{h^2}{2!} s_j^{(2r)} + \frac{h^3}{3!} s_{j_R}^{(2r+1)}$$

and

$$s_{j-1}^{(2r-2)} = s_j^{(2r-2)} - h\, s_{j_L}^{(2r-1)} + \frac{h^2}{2!} s_j^{(2r)} - \frac{h^3}{3!} s_{j_L}^{(2r+1)} .$$

Then the necessary and sufficient condition that $s_{j_R}^{(2r-1)} = s_{j_L}^{(2r-1)}$ at each interior point is that

$$\delta^2\, s_j^{(2r-2)} = h^2\, s_j^{(2r)} + \frac{h^2}{3!} \delta^2\, s_j^{(2r)} .$$

which is easily deduced from the preceding two equations and equation (2.1-1) .

If the above process is carried out for all even derivatives, then this complete set can be compactly written as

$$\delta^2\, s_j^{(2p)} = 2 \sum_{i=1}^{t} \frac{h^{2i}}{(2i)!}\, s_j^{(2i+2p)} + \frac{h^{2t}\delta^2 s_j^{(2r)}}{(2t+1)!} , \qquad p = 0,1,\ldots,r-1$$

(2.1-2)

where $t = r - p$. The equations (2.1-2) may be linearly combined to yield the further set

$$h^{2p} \delta^2 s_j^{(2p)} = h^{2+2p} s_j^{(2+2p)} + \sum_{i=1}^{t} a_i h^{2i+2p} \delta^2 s_j^{(2i+2p)} , \tag{2.1-3}$$

where the values a_i satisfy the equations

$$\frac{1}{(2s+2)!} = \sum_{k=1}^{s} \frac{a_k}{(2s-2k+2)!} , \qquad s = 1,2,\ldots,t-1 \tag{2.1-4}$$

and

$$a_t = \frac{1}{(2t+1)!} - \sum_{k=1}^{t-1} \frac{a_k}{(2t-2k+1)!} . \tag{2.1-5}$$

The advantage of working with the equations (2.1-3) rather than those given by (2.1-2) is that in their full form the former set is more diagonally dominant than the latter.

It is possible to express the quantities a_k , $k = 1,2,\ldots,t$, in terms of the Bernoulli numbers (Abramowitz and Stegun [1,p.804])* and simple manipulation gives

$$A_s = \frac{2s-1}{(2s)!} B_{2s}, \quad s = 1,2,\ldots,t-1 \tag{2.1-6}$$

and

$$a_s = \frac{B_{2s}}{(2s-1)!} . \tag{2.1-7}$$

The spline is not yet uniquely defined. There are $2r + 2$ unknowns in each interval of the partition and n intervals giving a total of $2rn + 2n$ unknowns. The equations (2.1-3) (which hold if and only if the odd derivatives $s_j^{(1)}$, $s_j^{(3)}$, ..., $s_j^{(2r-1)}$ are continuous

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* The first few Bernoulli numbers are $B_0=1$, $B_1=-\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_3 = 0$, $B_4 = \frac{-1}{30}$.

for $j = 1,2,\ldots,n-1$) only provide $r(n-1)$ conditions. The fact that even derivatives $s_j^{(0)}, s_j^{(2)}, \ldots, s_j^{(2r)}$ are continuous for $j = 1,2,\ldots,n-1$ gives $(r+1)(n-1)$ conditions and finally there are the $n + 1$ interpolation conditions $s_j = y_j$. A convenient way to obtain the $2r$ additional conditions needed to uniquely determine $s(x)$ is to assume that the even derivatives $s^{(2p)}$, $p = 1,2,\ldots,r$, are given at x_0 and x_n.

Uniqueness of the spline defined in terms of the first r even derivatives can be justified by using Polya's theorem (Schoenberg [33]) which implies as a particular case that a $2r + 1^{st}$ degree polynomial is uniquely defined over an interval, if its function values and first r even derivatives are known at the endpoints of the interval.

2.1.3 Matrix formulation of the equations defining the spline

It is natural to write the set of equations (2.1-3) as a block matrix linear system, where each block of the matrix is a tridiagonal block and the overall form of the matrix is block upper Hessenberg. Thus the equations (2.1-3) are, when written in their full form,

$$\begin{bmatrix} I+A_1T & -A_2T & A_3T & \cdots & (-1)^{r-2}A_{r-1}T & (-1)^{r-1}a_rT \\ T & I+A_1T & -A_2T & \cdots & (-1)^{r-3}A_{r-2}T & (-1)^{r-2}a_{r-1}T \\ & T & I+A_1T & \cdots & (-1)^{r-4}A_{r-3}T & (-1)^{r-3}a_{r-2}T \\ & & \ddots & \ddots & \vdots & \vdots \\ & \bigcirc & & & I+A_1T & -a_2T \\ & & & & T & I+a_1T \end{bmatrix} \quad r \times r$$

$$\begin{bmatrix} h^2\underline{s}^{(2)} \\ -h^4\underline{s}^{(4)} \\ h^6\underline{s}^{(6)} \\ \cdot \\ \cdot \\ \cdot \\ (-1)^{r-2}h^{2r-2}\underline{s}^{(2r-2)} \\ (-1)^{r-1}h^{2r}\underline{s}^{(2r)} \end{bmatrix} = \underline{b} , \qquad (2.1\text{-}8)$$

where $\underline{b}$ is a known vector depending on the known function values and boundary conditions: $\underline{s}^{(2)} = \{s_1^{(2)}, s_2^{(2)}, \ldots, s_{n-1}^{(2)}\}^T$ and $\underline{s}^{(4)}, \underline{s}^{(6)}, \ldots, \underline{s}^{(2r)}$ are similarly defined; and T is the square $n-1 \times n-1$ matrix

$$T = \begin{bmatrix} -2 & 1 & & \bigcirc \\ 1 & -2 & \ddots & \\ & \ddots & \ddots & 1 \\ \bigcirc & & 1 & -2 \end{bmatrix} .$$

Albasiny and Hoskins [6] have already studied the convergence properties of iterative methods of numerically solving the system (2.1-8) and a summary of their results for the block Jacobi, block Gauss-Seidel and block SOR matrices and the best relaxation parameter w_b in the SOR method are given in table 2.1-1 .

r	ρ_J	ρ_{GS}	ρ_{SOR}	w_b
2	.632	.400	.127	1.1270
3	.810	.636	.248	1.2274
4	.885	.760	.343	1.2954
5	.923	.831	.419	1.3444
6	.945	.875	.479	1.3812

Table 2.1-1

The spectral radii of iteration matrices and best w_b for large n .

An alternative method of solution is to transform the coefficient matrix of the system (2.1-8) using the following theorem into a block tridiagonal matrix . The properties of iterative methods of solution of this block tridiagonal matrix may be analysed easily.

Theorem 2.1-1

If A is a composite matrix with block property P and all the elements of A have property Q then there exists a permutation matrix H such that HAH^T is a composite matrix with block property Q whose elements each have property P . Properties P and Q may describe any configuration of zero elements in a given matrix, for example an upper triangular $n \times n$ matrix has the property that there is an $n \times n$ configuration of zero elements below the diagonal.

Proof

The transformation required is a block-element exchange and as the position of each element in a block matrix can be designated as element

(i,j) local to the block (k,ℓ) for some unique k,ℓ,i and j, it follows that this element is then moved to position (k,ℓ) of block (i,j). Suppose the matrix A is a block $n_1 x n_1$ matrix with submatrices of dimension $n_2 x n_2$, and is transformed into a matrix B which is a block $n_2 x n_2$ matrix with submatrices of dimension $n_1 x n_1$. If the positions in A, elements (i_1, j_1) in blocks (k,ℓ), are zero for $k = 1,2,\ldots,n_1$ and $\ell = 1,2,\ldots,n_1$ then in matrix B all the elements (k,ℓ) in blocks (i_1, j_1) will be zero. If the matrix A has a block (k_1, ℓ_1) in which each element (i,j) is zero, $i = 1,2,\ldots,n_2$ and $j = 1,2,\ldots,n_2$ then the matrix B will have a zero in the position element (k_1, ℓ_1) of each of its blocks.

The proof is completed by demonstrating that a permutation matrix H can be found such that $B = HAH^T$. Define the set $C = \{m;\ m = (i-1)\,n_2 + j,\ i\ \varepsilon(1,2,\ldots,n_1)$ and $j\ \varepsilon(1,2,\ldots,n_2)\}$. The set C has as elements the integers $(1,2,3,\ldots,n_1n_2)$ and there is an automorphism on C which associates the element $m = (i-1)n_2 + j$ with the element $m' = (j-1)n_1 + i$. Now let the matrix $H = (h_{ij})_{n_1n_2xn_1n_2}$ be defined by the rule

$$h_{ij} = \begin{cases} 1 & \text{if } i\ \varepsilon\ C \text{ and } j \text{ is the corresponding element in } C' \\ 0 & \text{otherwise.} \end{cases}$$

The matrix H is a permutation matrix which moves row i of block k in matrix A to row k of block i in the matrix HA. It is easily seen then that $B = HAH^T$. □

If the theorem 2.1-1 is applied to the matrix of the linear system (2.1-8) the resulting system is

$$A\underline{s} = \underline{c}$$

or in expanded form

$$\begin{bmatrix} H_1 & H_2 & & & \bigcirc \\ H_2 & H_1 & \ddots & & \\ & \ddots & \ddots & \ddots & H_2 \\ \bigcirc & & & H_2 & H_1 \end{bmatrix}_{n-1 \times n-1} \begin{bmatrix} \underline{s}_1 \\ \underline{s}_2 \\ \vdots \\ \underline{s}_{n-1} \end{bmatrix} = \underline{c} \qquad (2.1\text{-}9)$$

where $H_1 = I - 2\,H_2$,

$$H_2 = \begin{bmatrix} A_1 & -A_2 & A_3 & \cdots & (-1)^{r-1}a_r \\ 1 & A_1 & -A_2 & \cdots & (-1)^{r-2}a_{r-1} \\ & 1 & A_1 & \cdots & (-1)^{r-3}a_{r-2} \\ & & \ddots & \ddots & \vdots \\ \bigcirc & & & 1 & a_1 \end{bmatrix} \qquad (2.1\text{-}10)$$

and $\underline{s}_1 = \{h^2 s_1^{(2)}, -h^4 s_1^{(4)}, \ldots, (-1)^{r-1} h^{2r} s_1^{(2r)}\}$ and $\underline{s}_2, \underline{s}_3, \ldots,$ $\underline{s}_{n-1}$ are defined similarly and $\underline{c}$ is a known vector depending on given values.

The matrices H_1 and H_2 have special properties , given in the following two lemmas , which will be needed in subsequent developments.

<u>Lemma 2.1-1</u>

The spectral radius of H_2, i.e. $\rho(H_2)$, is less than 1/4 .

Proof

By the definition of A_s and a_s , H_2 is a matrix of non-negative elements. Let D be the diagonal matrix diag $(1, \pi^2 \alpha^2, \pi^4 \alpha^4, \ldots, \pi^{2r-2} \alpha^{2r-2})$ and consider the matrix $D^{-1}H_2D$, which is similar to H_2 . Gerschgorin's theorem (Varga [45,p.16]) may be used to bound $\rho(D^{-1}H_2D)$ in the following way.

In the first $r - 1$ columns of $D^{-1}H_2D$ the sum of the off-diagonal terms is certainly bounded by

$$\frac{1}{\pi^2 \alpha^2} + \sum_{n=2}^{\infty} (-1)^{n-1} A_n (\pi^2 \alpha^2)^{n-1} .$$

Using the definition for A_n $(A_n = \frac{2n-1}{(2n)!} B_{2n})$ the above equation thus may be written as

$$\frac{1}{\pi^2 \alpha^2} + \sum_{n=2}^{\infty} (-1)^{n-1} \frac{(2n-1)}{(2n)!} B_{2n} (\pi\alpha)^{2n-2} .$$

However, the generating function for the Bernoulli numbers is

$$\frac{x}{e^x-1} = \sum_{n=0}^{\infty} \frac{B_n x^n}{n!} \tag{2.1-11}$$

and upon division by x , differentiation with respect to x and substitution of $x = i\pi\alpha$ one has

$$\frac{1}{\pi^2 \alpha^2} + \sum_{n=2}^{\infty} (-1)^{n-1} \frac{2n-1}{(2n)!} B_{2n} (\pi\alpha)^{2n-2} = \frac{-1}{2(\cos\pi\alpha-1)} - \frac{1}{12} .$$

The diagonal element in the first $r - 1$ columns is 1/12 and a bound on $\rho(H_2)$ is $\frac{-1}{2(\cos\pi\alpha-1)}$, thus if α is taken to be unity , then the minimum bound is just $\frac{1}{4}$.

For the r^{th} column, the sum of the off-diagonal terms is bounded by

$$\sum_{n=2}^{\infty} (-1)^{n-1} a_n (\pi\alpha)^{2n-2} = \sum_{n=2}^{\infty} \frac{B_{2n}}{(2n-1)!} (i\pi\alpha)^{2n-2} .$$

Differentiating the series (2.1-11) and substituting $x = i\pi\alpha$ now gives

$$\sum_{n=2}^{\infty} \frac{B_{2n}}{(2n-1)!} (i\pi\alpha)^{2n-2} = \frac{-1}{2(\cos\pi\alpha-1)} - \frac{1}{2\pi\alpha} \cot \frac{\pi\alpha}{2} - \frac{1}{6} .$$

For $\alpha = 1$, this quantity is $\frac{1}{4} - \frac{1}{6}$, but since the diagonal element is just 1/6 , a bound on $\rho(H_2)$ is again less than 1/4 . Thus $\rho(H_2) < \frac{1}{4}$ for all r , which proves the lemma. □

Lemma 2.1-2

If $\rho(H_2) < \frac{1}{4}$ then H_1 is non-singular.

Proof

The matrix H_1 is defined as $I - 2H_2$, thus if λ_i is an eigenvalue of H_2 then $\mu_i = 1 - 2\lambda_i$ is an eigenvalue of H_1 . Simple inequalities then yield

$$|\mu_i| = |1 - 2\lambda_i| \geq |(1 - 2|\lambda_i|)| ,$$

but $\rho(H_2) < \frac{1}{4}$ so $|\lambda_i| < \frac{1}{4}$ and thus

$$|\mu_i| > |1 - 2 (\tfrac{1}{4})| = \frac{1}{2} .$$

and it follows that the matrix H_2 has no zero eigenvalues and H_1 is non-singular. □

2.2 Calculation of the optimal SOR parameter

Common iterative methods for solving linear systems of equations are discussed by Varga [45] , specifically the Jacobi method, the Gauss-Seidel method and the successive-overrelaxation (SOR) method are of interest here. For the system of equations $A\underline{x} = \underline{k}$, let D be the matrix of diagonal elements of A , let E be the negative lower triangular matrix of A and let F be the negative upper triangular matrix of A .

The Jacobi iteration is described by the equation

$$\underline{x}^{(m+1)} = B\underline{x}^{(m)} + D^{-1}\underline{k}$$

where m is the iteration index and $B = D^{-1}(E+F)$ is the point Jacobi matrix. The Gauss-Seidel iteration is described by the equation

$$\underline{x}^{(m+1)} = C\underline{x}^{(m)} + (D - E)^{-1}\,\underline{k}$$

where $C = (D - E)^{-1}\,F$ is the point Gauss-Seidel matrix. Letting $L = D^{-1}\,E$ and $U = D^{-1}\,F$ the SOR iteration is

$$\underline{x}^{(m+1)} = L_w\underline{x}^{(m)} + w\,(I - wL)^{-1}\,D^{-1}\,K$$

where $L_w = (I - wL)^{-1}\,[(1-w)I+wU]$ is the point SOR matrix. The quantity w is a relaxation parameter to be chosen before applying the SOR method.

The Jacobi method converges if $\rho(B) < 1$ where $\rho(B)$ is the spectral radius of the matrix B . The Gauss-Seidel method converges if $\rho(C) < 1$ and the SOR method converges if $\rho(L_w) < 1$. The closer $\rho(L_w)$ is to 0 the faster the SOR method will converge so w is usually chosen so as to minimize $\rho(L_w)$. Block iterative processes, and in particular, block Jacobi, block Gauss-Seidel and block SOR are defined analogously to the above point Jacobi, Gauss-Seidel and SOR methods with A being a block matrix. The following theorems make it possible to find the optimal SOR parameter, w_b, for the matrix A in equation (2.1-9).

Theorem 2.2-1 (Varga [45,p.109])

If A is a consistently ordered 2-cyclic matrix with non-singular diagonal submatrices and $\rho(B) < 1$ where B is the block Jacobi matrix then

$$w_b = \frac{2}{1 + \sqrt{(1 - \rho^2(B))}} ,$$

$$\rho(C) = \rho^2(B)$$

$$\rho(L_{w_b}) = w_b - 1 .$$

Theorem 2.2-2 (Varga [45,p.102])

If the diagonal submatrices of a block tridiagonal matrix are non-singular then the matrix is consistently ordered and 2-cyclic.

By lemma 2.1-2 the diagonal submatrices of the block tridiagonal-matrix A in equation (2.1-9) are non-singular, thus A is a consistently ordered 2-cyclic matrix. The following lemmas show that the matrix A satisfies all the conditions of theorem 2.2-1.

Lemma 2.2-1

The spectral radius of B, $\rho(B)$, is less than one for all n and r where B is the block Jacobi matrix associated with the matrix A in equation (2.1-9). The matrix B is defined by

$$B = \begin{bmatrix} 0 & -H_1^{-1}H_2 & & \bigcirc \\ -H_1^{-1}H_2 & 0 & \ddots & \\ & \ddots & \ddots & -H_1^{-1}H_2 \\ \bigcirc & & -H_1^{-1}H_2 & 0 \end{bmatrix}_{n-1 \times n-1} .$$

The eigenvalues of the matrix

$$\begin{bmatrix} 0 & 1 & & \bigcirc \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ \bigcirc & & 1 & 0 \end{bmatrix}_{n-1 \times n-1}$$

are known to be (Gregory and Karney [18]) $2 \cos \frac{\pi j}{n}$, $j = 1,2,\ldots,n-1$ and if μ_i , $i = 1,2,\ldots,r$ are the eigenvalues of the matrix $-H_1^{-1}H_2$, then by Afriat's theorem (Afriat [2]) the eigenvalues of B are $2\mu_i \cos \frac{\pi j}{n}$. Thus

$$\rho(B) = 2\rho(-H_1^{-1}H_2) \max_j \cos \frac{\pi j}{n}$$

$$= 2\rho(-H_1^{-1}H_2) \cos \frac{\pi}{n} .$$

Now, suppose λ_i are the eigenvalues of H_2 , then it follows that $-\lambda_i/(1 - 2\lambda_i)$ are the eigenvalues of $-H_1^{-1}H_2$ and since

$$\left|\frac{-\lambda_i}{1 - 2\lambda_i}\right| = \frac{|\lambda_i|}{|1 - 2\lambda_i|}$$

$$\leq \frac{|\lambda_i|}{|(1 - 2|\lambda_i|)|} ,$$

then from lemma 2.1-1, $|\lambda_i| < \frac{1}{4}$, and it can be concluded that

$$\frac{|\lambda_i|}{|(1 - 2|\lambda_i|)|} < \frac{1}{2}$$

and

$$\rho(-H_1^{-1}H_2) < \frac{1}{2} .$$

Finally the spectral norm of B , i.e. $\rho(B)$, is less than $2(\frac{1}{2}) \cos \frac{\pi}{n}$ which is less than 1 . □

It is interesting to note that this lemma proves that the iterative methods converge for all n and r . In the following table some numerical values for $\rho(B)$ for various values of r and using theorem 2.1-1 are detailed.

r	$\rho(B)$	$\rho(C)$	$\rho(L_{w_b})$	w_b
2	.7265	.5278	.1854	1.1854
3	.8321	.6924	.2865	1.2865
4	.8878	.7882	.3697	1.3697
5	.9202	.8467	.4373	1.4373
6	.9405	.8845	.4927	1.4927
7	.9540	.9101	.5386	1.5386
8	.9634	.9281	.5771	1.5771

Table 2.2-1

The spectral radii of iteration matrices and best w_b for large n .

Chapter 3

Error analysis and some applications of cubic multiple spline approximations

3.1 Definition and uses of cubic multiple splines

It is well-known that if a spline is used to approximate a given function which has sufficiently many continuous derivatives, then the derivatives of the spline approximate the corresponding derivatives of the function with a fair degree of accuracy. Asymptotic bounds for the differences between the cubic spline estimates of various derivatives of the function being approximated and the exact values have been discussed in the literature and explicit bounds are given by Hall [20] . If the function being approximated has sufficiently many continuous derivatives, then under some boundary conditions improved estimates for the second derivatives can be obtained by fitting a cubic spline to the first derivatives of the interpolating cubic spline. This technique is called spline on spline or multiple spline interpolation and was first suggested and demonstrated numerically by Ahlberg et al. [4,p.48] .

This chapter establishes that for periodic cubic splines defined on a uniform partition a multiple spline gives more accurate values for the second derivative of the function than does the usual spline approximation. The multiple spline approximation of the second derivative of a given function for both periodic and non-periodic splines defined on uniform and non-uniform partitions is investigated. Multiple splines are then, for purely illustrative purposes, used to solve a boundary value problem.

3.2 Error analysis of the approximation of second derivatives of a function using cubic splines and cubic multiple splines

3.2.1 Notation

If $g(x)$ is a function defined on an interval $[x_0, x_n]$, $\|g\| = \max_{x \in [x_0, x_n]} |g(x)|$, and when A is an $n \times n$ matrix with elements a_{ij} then $\|A\| = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$. The term $\text{circ}(a_1, a_2, \ldots, a_n)$ denotes an $n \times n$ circulant matrix with first row $(a_1, a_2, \ldots, a_n)$ while $\text{diag}(a_1, a_2, \ldots, a_n)$ is a diagonal matrix with the quantities $a_1, a_2, \ldots, a_n$ appearing on the main diagonal. The abbreviations s_j, s'_j, s''_j and y_j, y'_j, y''_j are taken to mean $s(x_j)$, $s'(x_j)$, $s''(x_j)$ and $y(x_j)$, $y'(x_j)$, $y''(x_j)$ respectively.

A cubic spline $s(x)$ interpolating to a function $y(x)$ on an interval $[x_0, x_n]$ is a piecewise polynomial which passes through the $n + 1$ points (x_j, y_j), $j = 0,1,\ldots,n$, where the points x_j form a partition of $[x_0, x_n]$. The positive quantities h_j are defined as $x_j - x_{j-1}$, $j = 1,2,\ldots,n$, while $\underline{h} = \min_j h_j$ and $\overline{h} = \max_j h_j$. The analysis parallels the work of Kershaw [29] where the error in approximation of the first derivative of a function by a cubic spline with various boundary conditions is given.

3.2.2 Approximation of the second derivative of a non-periodic function

In this section the second derivative is approximated by both cubic splines and cubic multiple splines using the boundary conditions that first and second derivatives of the function are known at the end-points of $[x_0, x_n]$. It is determined that approximation by periodic cubic multiple splines is two orders of h more accurate than approximation by cubic splines when the splines are defined on a uniform partition with spacing h and numerical results are given to support this case.

Let the cubic spline $s(x)$ interpolate to the function $y(x)$ as above and let the elements of the $n-1 \times n-1$ matrices A and B be

$$a_{ij} = \begin{cases} \lambda_i & j = i + 1 \\ 2 & j = i \\ \mu_i & j = i - 1 \\ 0 & \text{otherwise} \end{cases}$$

and

$$b_{ij} = \begin{cases} 6\lambda_i/h_{i+1}^2 & j = i + 1 \\ -6/(h_i h_{i+1}) & j = i \\ 6\mu_i/h_i^2 & j = i - 1 \\ 0 & \text{otherwise} \end{cases}$$

respectively where

$$\lambda_i = h_{i+1}/(h_i + h_{i+1})$$

and

$$\mu_i = 1 - \lambda_i \, , \qquad i = 1,2,\ldots,n-1 \, .$$

The equations defining the spline $s(x)$ are then

$$A\underline{s}'' = B\underline{y} + \underline{b} \qquad (3.2\text{-}1)$$

where $\underline{s}'' = \{s_1'', s_2'', \ldots, s_{n-1}''\}^T$, $\underline{y} = \{y_1, y_2, \ldots, y_{n-1}\}^T$ and

$\underline{b} = \{-\mu_1 y_0'', 0, \ldots, 0, -\lambda_{n-1} y_n''\}^T$ (Ahlberg et al [4]). Expansion of the function $y(x)$ using Taylor's theorem then gives the result

$$A\underline{y}'' = B\underline{y} + \underline{b} + \underline{v} \qquad (3.2\text{-}2)$$

where $\underline{v}$ is a vector with elements

$$v_j = \frac{1}{4}(h_j^3 + h_{j+1}^3)/(h_j + h_{j+1})\, y^{iv}(\xi_j)$$

with $\xi_j \in [x_{j-1}, x_{j+1}]$, $j = 1,2,\ldots,n-1$. However, A is diagonally dominant and hence non-singular while $\|A^{-1}\| \le 1$ (Hall [20]), thus equations (3.2-1) and (3.2-2) may be combined with the inequality $h_j^3 + h_{j+1}^3 \le \bar{h}^2 (h_j + h_{j+1})$ to give

$$|y_j'' - s_j''| \le \frac{1}{4}\bar{h}^2 \|y^{iv}\| \qquad j = 1,2,\ldots,n-1 . \qquad (3.2\text{-}3)$$

The inequality (3.2-3) therefore gives a bound on the error made in approximating the second derivative of a function $y(x)$ by a cubic spline.

Now suppose that the function $y(x)$ is to be approximated on $[x_0, x_n]$ by a cubic multiple spline. Let $s(x)$ be the cubic spline interpolating to the points (x_j, y_j) , $j = 0,1,\ldots,n-1$ where the x_j are not necessarily equally spaced and let $t(x)$ be the cubic spline interpolating to the points (x_j, s_j'), $j = 0,1,\ldots,n-1$. The equations defining these two splines are

$$C\underline{s}' = D\underline{y} + \underline{c}$$

and (3.2-4)

$$C\underline{t}' = D\underline{s}' + \underline{d}$$

where C and D are n-1 x n-1 matrices with elements

$$c_{ij} = \begin{cases} \mu_i & j = i + 1 \\ 2 & j = i \\ \lambda_i & j = i - 1 \\ 0 & \text{otherwise} \end{cases}$$

and

$$d_{ij} = \begin{cases} 3\mu_i/h_{i+1} & j = i + 1 \\ 3\lambda_i/h_i - 3\mu_i/h_{i+1} & j = i \\ -3\lambda_i/h_i & j = i - 1 \\ 0 & \text{otherwise} \end{cases}$$

and the vectors $\underline{c}$ and $\underline{d}$ are

$$\underline{c} = \{-\lambda_1\, y_0',\ 0,\ \ldots,\ 0,\ \mu_{n-1}\, y_n'\}^T$$

and

$$\underline{d} = \{-\lambda_1\, y_0'',\ 0,\ \ldots,\ 0,\ \mu_{n-1}\, y_n''\}^T$$

Expansion of $y(x)$ and $y'(x)$ using Taylor's theorem gives the results

$$C\underline{y}' = D\underline{y} + \underline{c} + \underline{v}$$

and (3.2-5)

$$C\underline{y}'' = D\underline{y}' + \underline{d} + \underline{w}$$

where the vectors $\underline{v}$ and $\underline{w}$ have components (Hall [20]),

$$v_j = \frac{1}{24} \frac{h_j h_{j+1}^3 + h_{j+1} h_j^3}{h_j + h_{j+1}} y^{iv} (\theta_j)$$

and

$$w_j = \frac{1}{24} \frac{h_j h_{j+1}^3 + h_{j+1} h_j^3}{h_j + h_{j+1}} y^{v} (\phi_j)$$

with θ_j and $\phi_j \in [x_{j-1}, x_{j+1}]$, $j = 1,2,\ldots,n-1$. From equations (3.2-4) and (3.2-5) it is easy to deduce that

$$\underline{y}'' - \underline{t}' = C^{-1} D C^{-1} \underline{v} + C^{-1} \underline{w} .$$

However, $\|D\| \le 3/\underline{h} (\bar{h}/\underline{h})$ and $\|C^{-1}\| \le 1$ (Hall [20]) and so taking norms on both sides of the above equation yields

$$|y_j'' - t_j'| \le \frac{1}{8} (\bar{h}/\underline{h})^2 \bar{h}^2 \|y^{iv}\| + \frac{1}{24} \bar{h}^3 \|y^{v}\| \qquad j = 1,2,\ldots,n-1 . \qquad (3.2\text{-}6)$$

A comparison of equations (3.2-3) and (3.2-6) shows that the multiple spline approximation and the ordinary spline approximation of the second derivative are of the same order of $\bar{h}$ when the splines are defined on unequally spaced knots.

The above analysis is simpler and an improvement in accuracy is observed, if the cubic splines are defined on a uniform partition with spacing h . If the defining equations for the spline are as in equation (3.2-1) given by