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A spline shooting technique for two point boundary value problems

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TABLE OF CONTENTS

I. INTRODUCTION

In this paper we consider the two point boundary value problem in ordinary differential equations

$$y'' = f(x,y),\ y(a) = A,\ y(b) = B. \tag{1.1}$$

Our purpose will be to study the application of cubic spline functions to the numerical treatment of (1.1). That is, we develop a method which produces a cubic spline function approximation to the analytical solution of (1.1) over the finite interval $[a,b]$. Some remarks concerning the applicability of our method in solving the general two point boundary value problem

$$y'' = f(x,y,y'),\ y(a) = A,\ y(b) = B, \tag{1.2}$$

will be made in Chapter VII.

Before we consider a numerical method for solving (1.1), we must be assured that there exists a unique analytical solution. The following class of boundary value problems defined by Henrici [6, p.347] is fundamental to this problem.

<u>Definition 1.1</u>: A boundary value problem will be said to be of class M if it is of the form (1.1) where

$-\infty < a < b < \infty$, A and B are arbitrary constants, and the function $f(x,y)$ satisfies the following conditions:

(i) $f(x,y)$ is defined and continuous in the infinite strip $T = \{(x,y) : a \leq x \leq b, -\infty < y < \infty\}$;

(ii) $f(x,y)$ satisfies a Lipschitz condition in y uniformly in x, that is, there exists a constant L such that for any $x \in [a,b]$ and any two numbers y and y^*,

$|f(x,y) - f(x,y^*)| \leq L|y - y^*|$;

(iii) $f_y(x,y)$ is continuous and nonnegative in T.

Problems of class M are nice in the following sense:

Theorem 1.1: A boundary value problem of class M has a unique solution. The proof of this theorem can be found in [6, p.347]. In this paper we will only consider problems of class M so that the solution $y(x)$ of (1.1) exists and is unique.

There is an extensive literature on the numerical solution of (1.1). Although existence of unique solutions for the two point boundary value problem has been established under fairly general conditions, there are no general methods for finding the solutions analytically. In fact Henrici [6, p.2] points out that even relatively innocent-looking differential equations, such as $y'' = 6y^2 + x$, cannot be solved in terms of elementary functions. Furthermore, even in cases where an explicit solution does exist, the problem of finding its numerical values may be difficult as for example in the solution $e^{-x^2}\int_0^x e^{t^2}dt$ of the equation $y'' = 4x^2y - 2(x+1)$, $y(0) = 0$, $y(1) = \frac{1}{e}\int_0^1 e^{t^2}dt$. It is important to have practical methods for approximating the solution of (1.1) with arbitrarily high accuracy. The advent of the high-speed digital computer has made the use of numerical methods for solving (1.1) not only feasible but also very attractive.

The known numerical methods generally fall into two categories:

(i) discrete variable methods which produce a table of approximate values at usually equidistant points of the independent variable, and

(ii) global (continuous) methods which produce a continuous approximating function over the entire interval $[a,b]$.

Concerning the first type, Chapter VII in Henrici [6] contains applications of such methods to our problem (1.1), along with an extensive bibliography. In particular he notes that it is theoretically always possible to reduce the solution of (1.1) to the solution of a sequence of initial value problems. Let $y(x,s)$ denote the solution of the initial value problem resulting from (1.1) by replaceing the condition for $y(b)$ by the condition $y'(a) = s$, where s is a parameter. Then (1.1) is equivalent to solving the (in general nonlinear) equation $y(b,s) = B$ for the solution $s = s^*$. This can be accomplished by one of the standard methods such as regula falsi or Newton's method, however, each evaluation of the function $y(x,s)$ (and, if Newton's method is used, of $y_s(x,s)$) requires the solution of an initial value problem. That is, one starts with an initial slope s_o and sees what happens at $x = b$ by solving the associated initial value problem. A "better" slope s_1 is generated using this information and the process is repeated. Continuing in this fashion a sequence of slopes $\{s_n\}$ is generated with the hope that $s_n \to s^*$ as $n \to \infty$. Chapter II in Keller [7] contains some general results concerning this so-called "shooting" or "drive-through" technique wherein the associated initial value problems are solved using a stable discrete variable method of order p.

Our interest is in using the "shooting" technique to construct a global or continuous approximation to the solution. The approach we take leads to the subject of spline functions, the first mention of which was made by Schoenberg [10]. The following definition is due to him.

<u>Definition 1.2</u>: Suppose we are given a sequence of real numbers

$$a = x_o < x_1 < \cdots < x_n = b. \tag{1.3}$$

A function $S(x)$ is a spline function of degree $m \geqq 1$ if it satisfies:

(i) $S(x) \in C^{m-1}[a,b]$;

(ii) $S(x) \in \pi_m$ in each subinterval (x_i, x_{i+1}), $i = 0,1,\ldots,n-1$, where π_m is the set of all polynomials of degree $\leqq m$. The points (1.3) are called knots (sometimes joints or mesh points) of the spline $S(x)$ and may be jump discontinuities of $S^{(m)}(x)$.

Note that $\pi_m \subset \mathcal{S}_m$, where $\mathcal{S}_m$ denotes the set of all spline functions of degree m, class $C^{m-1}[a,b]$.

A recent study on the application of spline functions for approximating the solution of the initial value problem

$$y' = f(x,y), \; y(a) = y_o \tag{1.4}$$

has been done by Loscalzo and Talbot [8]. Some of the ideas behind their construction of the spline function approximation will be implemented here.

As before, we replace (1.1) by the initial value problem

$$y'' = f(x,y), \; y(a) = A, \; y'(a) = s \tag{1.5}$$

where s is a parameter. A cubic spline function, which we will denote by $S(x,s)$, is generated to approximate the solution $y(x,s)$ of (1.5). We use a Taylor expansion of order two at $x = x_o$ and define the coefficient a_1 of x^3 by a collocation requirement at $x = x_1 = x_o + h$

$$S''(x_1,s) = f(x_1,S(x_1,s)).$$

A similar Taylor expansion at $x = x_1$ yields the first three coefficients of the next polynomial component of degree 3, and a collocation condition at $x = x_2 = x_o + 2h$ gives the fourth coefficient a_2 and completes the definition up to the determination of s. This process is repeated until of spline function of degre $m = 3$ is defined in terms of s over the entire range of integration $[a,b]$ with knots $x_i = a + ih$, $i = 1,2,\ldots,n-1$ and $h = (b-a)/n$. For the determination of the parameter s we require that the spline function $S(x,s)$ satisfy the boundary condition at $x = b$:

$$S(b,s) = B. \qquad (1.6)$$

This completes the definition of $S(x,s)$. As one might suspect, the initial slope s, determined by equation (1.6), can be written as a function of the coefficients a_i, $i = 1,\ldots,n$. Note also that $S(x,s)$ has two continuous derivatives for $x \varepsilon [a,b]$.

Loscalzo and Talbot [8] discovered that any spline function in $\mathcal{S}_m$ with equidistant knots satisfies a linear consistency relation which is equivalent to a discrete multistep method if it is applied to the initial value problem (1.4). Similarly, we find that such a spline function is equivalent to a discrete multistep method if it is applied to the boundary value problem (1.1).

II. CONSTRUCTION OF THE CUBIC SPLINE FUNCTION

Consider the boundary value problem of class M:

$$y'' = f(x,y) \tag{2.1}$$

$$y(a) = A, \ y(b) = B \tag{2.2}$$

Let $y(x,s)$ denote the solution of the initial value problem resulting from (2.1) and (2.2) by replacing the condition for $y(b)$ by the condition $y'(a) = s$, where s is a parameter:

$$y'' = f(x,y) \tag{2.3}$$

$$y(a) = A, \ y'(a) = s. \tag{2.4}$$

We wish to determine an initial slope s so that the approximate solution $S(x,s)$, which we will construct, to $y(x,s)$ will also be a good approximation to the solution $y(x,s^*)$ of (2.1); here s^* is the solution of the equation $y(b,s) = B$.

Our construction is as follows. Let $n > 3$ be an integer, $h = \frac{b-a}{n}$, and let $S(x,s)$ $(a \leqq x \leqq b)$ be a spline function of degree 3, class C^2 and having its knots at the points $x = a + h, a + 2h, \ldots, a + (n-1)h$. We define the first component of $S(x,s)$ by

$$\begin{aligned} S(x,s) &= y(a,s) + y'(a,s)(x-a) + \frac{1}{2!} y''(a,s)(x-a)^2 \\ &\qquad + \frac{1}{3!} a_1 (x-a)^3 \\ &= A + s(x-a) + \frac{1}{2} f(a,A)(x-a)^2 + \frac{1}{6} a_1 (x-a)^3, \\ &\qquad a \leq x \leq a+h \end{aligned} \tag{2.5}$$

with the last coefficient a_1 and, of course, the slope s as yet undetermined. We now require that $S(x,s)$ satisfy (2.3) for $x = a + h$. This gives the equation

$$S''(a+h,s) = f(a+h, S(a+h,s)). \tag{2.6}$$

More explicitly we have,

$$S(a+h,s) = A + sh + \frac{1}{2} f(a,A)h^2 + \frac{1}{6} a_1 h^3$$

$$S''(a+h,s) = f(a,A) + a_1 h,$$

so that (2.6) becomes

$$a_1 = \frac{1}{h}[f(a+h, A+sh+\frac{1}{2}f(a,A)h^2+\frac{1}{6}a_1h^3) - f(a,A)]$$
$$= g_1(s,a_1). \tag{2.7}$$

Repeating the same steps in the interval $[a+h, a+2h]$, we define

$$S(x,s) = \sum_{k=0}^{2} \frac{1}{k!} s^{(k)}(a+h,s)[x-(a+h)]^k$$
$$+ \frac{1}{3!} a_2[x-(a+h)]^3 \tag{2.8}$$

and require $S(x,s)$ to satisfy (2.3) at $x = a + 2h$

$$S''(a+2h,s) = f(a+2h, S(a+2h,s)). \tag{2.9}$$

This results in the equation

$$a_2 = \frac{1}{h}[f(a+2h, A+2sh+2f(a,A) + \frac{7}{6}a_1h^3 + \frac{a_2h^3}{6})$$
$$- a_1h - f(a,A)] \tag{2.10}$$
$$= g_2(s,a_1,a_2).$$

Continuing in this manner we obtain a cubic spline function $S(x,s)$ satisfying the equations

$$S''(a+ih,s) = f(a+ih, S(a+ih,s)), \quad i = 0,1,\ldots,n \tag{2.11}$$

which results in the system of n nonlinear equations in the $n+1$ unknowns $a_1, a_2, \ldots, a_n, s$, that is

$$a_i = g_i(s, a_1, a_2, \ldots, a_i).$$

Now for the determination of the parameter s, we require that the spline function satisfy the boundary condition at $x = b$:

$$S(b,s) = B. \tag{2.12}$$

We have the following fact concerning the solution s of equation (2.12).

<u>Theorem 2.1</u>: If we require the cubic spline function constructed above to satisfy the boundary condition at $x = b$, the parameter s satisfies the equation

$$s = \frac{1}{b-a}\left[B - A - \frac{(b-a)^2}{2} f(a,A) - \frac{h^3}{3!} \sum_{j=1}^{n} c_j^n a_j\right] \qquad (2.13)$$

where $c_j^n = [n-(j-1)]^3 - [n-j]^3$.

The proof of this theorem relies on the following lemma:

<u>Lemma 2.2</u>: At the points $x = a + ih$, $i = 0,1,\ldots,n$, the cubic spline function $S(x,s)$ and its first two derivatives satisfy the equations:

$$S(a+ih,s) = A + ihs + \frac{(ih)^2}{2} f(a,A) + \frac{h^3}{3!} \sum_{j=1}^{i} c_j^i a_j \qquad (2.14)$$

$$S'(a+ih,s) = s + ihf(a,A) + h^2 \sum_{j=1}^{i} (i-j+\tfrac{1}{2}) a_j \qquad (2.15)$$

$$S''(a+ih,s) = f(a,A) + h \sum_{j=1}^{i} a_j \qquad (2.16)$$

<u>Proof of Lemma 2.2</u>: We will establish (2.14)-(2.16) by induction. Clearly, by construction, (2.16) holds for $i = 0$. Assume it is true for $i - 1$. Now over the interval $[a+(i-1)h, a+ih]$, $S(x,s)$ is given by

$$S(x,s) = \sum_{k=0}^{2} \frac{1}{k!} S^{(k)}(a+(i-1)h)[x-(a+(i-1)h)]^k$$

$$+ \frac{1}{3!} a_i[x-(a+(i-1)h]^3. \tag{2.17}$$

Hence $S'(x,s)$ and $S''(x,s)$ are given by

$$S'(x,s) = S'(a+(i-1)h,s) + S''(a+(i-1)h,s)[x-(a+(i-1)h)]$$

$$+ \frac{1}{2} a_i[x-(a+(i-1)h)]^2 \tag{2.18}$$

$$S''(x,s) = S''(a+(i-1)h,s) + a_i[x-(a+(i-1)h)]. \tag{2.19}$$

Now since (2.16) is assumed true for $i-1$,

$$S''(x,s) = f(a,A) + h \sum_{j=1}^{i-1} a_j + a_i[x-(a+(i-1)h],$$

and evaluating $S''(x,s)$ at $x = a+ih$ we find

$$S''(a+ih,s) = f(a,A) + h \sum_{j=1}^{i} a_j.$$

This proves (2.16).

To prove (2.15), we note that it is true for $i = 0$ by construction. Assume it is true for $i - 1$. Evaluating equation (2.18) at $x = a + ih$ we find

$$S'(a+ih,s) = S'(a+(i-1)h,s) + S''(a+(i-1)h,s)h + \frac{1}{2}h^2 a_i$$

$$= s + (i-1)hf(a,A) + h^2 \sum_{j=1}^{i-1} (i-1-j+\tfrac{1}{2})a_j$$

$$+ hf(a,A) + h^2 \sum_{j=1}^{i-1} a_j + \frac{1}{2}h^2 a_i$$

$$= s + ihf(a,A) + h^2 \sum_{j=1}^{i} (i-j+\tfrac{1}{2})a_j .$$

This proves (2.15).

Finally, to prove (2.14), we note that it is also true for $i = 0$ by construction. Assume it is true for $i - 1$. Evaluating equation (2.17) at $x = a + ih$ results in

$$S(a+ih,s) = S(a+(i-1)h,s) + hS'(a+(i-1)h,s)$$

$$+ \frac{h^2}{2} S''(a+(i-1)h,s) + \frac{1}{6} a_i h^3$$

$$= A + (i-1)hs + \frac{(i-1)^2}{2} h^2 f(a,A)$$

$$+ \frac{h^3}{G} \sum_{j=1}^{i-1} C_j^{i-1} a_j$$

$$+ hs + (i-1)h^2 f(a,A) + h^3 \sum_{j=1}^{i-1} (i-1-j+\tfrac{1}{2}) a_j$$

$$+ \frac{h^2}{2} f(a,A) + \frac{h^3}{2} \sum_{j=1}^{i-1} a_j + \frac{1}{6} a_i h^3$$

$$= A + ihs + \frac{(ih)^2}{2} f(a,A) + \frac{h^3}{3!} \sum_{j=1}^{i} C_j^i a_j .$$

This establishes equation (2.14).

<u>Proof of Theorem 2.1</u>: This follows directly from Lemma 2.2 by letting $i = n$. We have

$$S(a+nh,s) = S(b,s) = A + (b-a)s + \frac{(b-a)^2}{2} f(a,A)$$

$$+ \frac{h^3}{3!} \sum_{j=1}^{n} C_j^n a_j ,$$

and setting $S(b,s) = B$ and solving for the parameter s establishes equation (2.13).

Next we concern ourselves with the questions of existence and uniqueness of the cubic spline function constructed above. Recall that over the interval $[x_{i-1}, x_i]$ we define

$$S(x,s) = \sum_{k=0}^{2} \frac{1}{k!} S^{(k)}(x_{i-1},s)[x - x_{i-1}]^k + \frac{1}{3!} a_i[x - x_{i-1}]^3.$$

But from Theorem 2.1 we have the parameter s expressed in terms of the coefficients a_i, $i = 1,2,\ldots,n$, and hence because of the spline continuity conditions we see that $S(x,s)$ will be uniquely determined if the vector $\bar{a} = (a_1,a_2,\ldots,a_n)^T$ can be found uniquely.

Now the coefficients a_i are to be found from the collocation requirement

$$S''(x_i,s) = f(x_i,S(x_i,s)), \; i = 1,\ldots,n,$$

which by Lemma 2.2 becomes

$$f(a,A) + h \sum_{j=1}^{i} a_j = f(x_i,S(x_i,s)), \; i = 1,\ldots,n.$$

Solving for a_i we find

$$a_i = \frac{1}{h}[f(x_i,S(x_i,s)) - h\sum_{j=1}^{i-1} a_j - f(a,A)]$$

$$= \frac{1}{h}[f(x_i,S(x_i,s)) - S''(x_{i-1},s)]$$

$$= \frac{1}{h}[f(x_i,S(x_i,s)) - f(x_{i-1},S(x_{i-1},s))]$$

$$\equiv g_i(a_1,a_2,\ldots,a_n),\ i = 1,2,\ldots,n. \tag{2.20}$$

Hence if we denote by $\bar{a}$ the vector $\bar{a} = (a_1,\ldots,a_n)^T$, and by $\bar{g}$ the vector $\bar{g} = (g_1,\ldots,g_n)^T$, we see that the problem of finding the coefficients a_i, $i = 1,\ldots,n$, results in the solution of a system of (in general nonlinear) equations which in vector notation can be written

$$\bar{a} = \bar{g}(\bar{a}). \tag{2.21}$$

It is known [9,p.125] that if the Jacobian matrix U of $\bar{g}$, $U = \left(\frac{\partial g_j(\bar{a})}{\partial a_i}\right)$ satisfies the condition $\|U\| < 1$, where $\|\cdot\|$ denotes the spectral norm of $\cdot$, then $\bar{g}$ is a contraction mapping and the system (2.21) has a unique fixed point which may be found by iteration.

The elements of the matrix $U = (u_{ij})$ are explicity

$$u_{ij} = \frac{h^2}{6}\Big\{f_y(x_i,S(x_i,s))\Big[c_j^i - \frac{i}{n}c_j^n\Big]$$

$$- f_y(x_{i-1},S(x_{i-1},s))\Big[c_j^{i-1} - \frac{(i-1)}{n}\, c_j^n\Big]\Big\},$$

with c_ℓ^k as previously defined except for the condition $c_\ell^k = 0$ if $k < \ell$. Now if we define the matrix $T = (t_{ij})$ where $t_{ij} = \begin{cases} 1, & j \le i \\ 0, & j > i \end{cases}$, then $T^{-1} = (t_{ij}^{(-1)})$ where

$t_{ij}^{(-1)} = \begin{cases} 1, & j = i \\ -1, & j = i-1, \\ 0, & \text{otherwise} \end{cases}$ and $T\,U\,T^{-1} = P = (p_{ij})$ where

$$p_{ij} = \begin{cases} (b-a)^2 f_y(x_i,S(x_i,s))\Big[\dfrac{j(i-n)}{n^3}\Big], & j < i \\[2ex] (b-a)^2 f_y(x_i,S(x_i,s))\Big[\dfrac{6i^2-6in+n}{6n^3}\Big], & j = i < n \\[2ex] 0 & i = j = n \\[2ex] (b-a)^2 f_y(x_i,S(x_i,s))\Big[\dfrac{i(j-n)}{n^3}\Big], & i < j < n \\[2ex] (b-a)^2 f_y(x_i,S(x_i,s))\Big[\dfrac{i}{6n^3}\Big], & i < j = n\,. \end{cases}$$

Then, since $U = T^{-1}PT$, we have

$$\|U\| = \|T^{-1}PT\| \leq \|T^{-1}\|\|P\|\|T\| = \|P\| \tag{2.22}$$

as $\|T^{-1}\| = \|T\| = 1$.

Next we define the matrix $R = (r_{ij})$ where

$r_{ij} = \begin{cases} 1, & j = i \\ -\frac{1}{6}, & j = n,\ i = n-1 \\ 0, & \text{otherwise} \end{cases}$ from which we easily see that

$R^{-1} = (r_{ij}^{(-1)})$ is given by $r_{ij}^{(-1)} = \begin{cases} 1, & j = i \\ \frac{1}{6}, & j = n,\ i = n-1. \\ 0, & \text{otherwise} \end{cases}$

Performing another transformation we get $RPR^{-1} = Q_{f_y} = (q_{ij})$ where

$$q_{ij} = \begin{cases} (b-a)^2 f_y(x_i, S(x_i,s))\left[\frac{j(i-n)}{n^3}\right], & j < i \\ (b-a)^2 f_y(x_i, S(x_i,s))\left[\frac{6i^2 - 6in + n}{n^3}\right], & j = i < n \\ (b-a)^2 f_y(x_i, S(x_i,s))\left[\frac{i(j-n)}{n^3}\right], & j > i \end{cases}.$$

Note that $q_{ij} \leq 0$, $1 \leq i, j \leq n$ since $f_y \geq 0$.

For a given matrix A if we denote the spectral radius of A by $\rho(A)$ and the conjugate transpose of A by A^*, then since $P = R^{-1}Q_{f_y}R$ we get

$$\|P\| = \|R^{-1}Q_{f_y}R\| \leq \|R^{-1}\|\|Q_{f_y}\|\|R\| = \|Q_{f_y}\| \tag{2.23}$$

as $\|R^{-1}\| = \|R\| = 1.$

By definition,

$$\|Q_{f_y}\| = \left[\rho\left(Q^*_{f_y} Q_{f_y}\right)\right]^{\frac{1}{2}} \tag{2.24}$$

Observe that $Q^*_{f_y} Q_{f_y}$ is a nonnegative matrix and so if we assume $f_y \leq N$, and denote by Q_N the matrix resulting by replacing f_y by this upper bound in each component of the matrix Q_{f_y}, we have that

$$\rho\left(Q^*_{f_y} Q_{f_y}\right) \leq \rho\left(Q^*_N Q_N\right) = \left[\rho\left(Q_N\right)\right]^2, \tag{2.25}$$

as Q_N is symmetric. On combining equation (2.24) with inequalities (2.22), (2.23), and (2.25) we get that

$$\|U\| \leq \rho(Q_N). \tag{2.26}$$

Thus the system (2.21) has a unique fixed point when $\rho(Q_N) < 1$. Now the matrix $Q_N = (b-a)^2 N \cdot D$ where $D = (d_{ij})$ is given by

$$d_{ij} = \begin{cases} j(i-n)/n^3 & j < i \\ (6i^2 - 6in + n)/n^3, & j = i < n \\ i(j-n)/n^3 & j > i \\ 0 & i = j = n \end{cases},$$

and so we need to analyse $\rho(D)$. This was done for several values of n by finding the eigenvalues of the matrix D using the Power method and a computer. The results are listed in the following table.

Table 2.1

The spectral radius of D

n	$\rho(D)$
4	0.09627751
5	0.09805469
6	0.09903845
7	0.09963777
8	0.10002920
9	0.10029867
10	0.10049198
20	0.10111311
30	0.10122864
40	0.10126912

Now the condition that $\rho(Q_N) < 1$ is equivalent to requiring $N(b-a)^2\rho(D) < 1$. We conjecture that $\rho(D) < \frac{1}{\pi^2}$ and in fact that $\lim\limits_{n \to \infty} \rho(D) = \frac{1}{\pi^2}$. Note that $\frac{1}{\pi^2} \approx 0.10132118$ and that our results in Table 2.1 support this conjecture.

Finally it is interesting to note that if $\rho(D) < \frac{1}{\pi^2}$, then the condition under which system (2.21) has a unique fixed point is $N < \pi^2/(b-a)^2$. This agrees very well with a result in [1,p.31] which states that the boundary value problem (2.1)-(2.2) has a unique solution when $L < \pi^2/(b-a)^2$, and that this result is the best possible. Here L is a Lipschitz constant for the function f.

Throughout the rest of this paper it will be assumed that $b - a$ is small enough so that $\rho(Q_N) < 1$ which will guarantee existence of a unique solution to system (2.21).

In conclusion, suppose that we approximate the solution of system (2.21) by generating a sequence of vectors $\{\bar{a}^{(m)}\}$ through the algorithm

$$\bar{a}^{(m+1)} = \bar{g}(\bar{a}^{(m)}), \quad m = 0,1,\ldots\ .$$

Choosing $\bar{a}^{(0)} = \bar{0}$ admits the following rationale:

Consider the Taylor series expansion of the exact solution $y(x) \equiv y(x,s^*)$ of (1.1):

$$y(b) = y(a+nh) = y(a) + (b-a)y'(a) + \frac{(b-a)^2}{2}y''(a) + \cdots$$

or

$$B = A + (b-a)s^* + \frac{(b-a)^2}{2}f(a,A) + \cdots .$$

Upon solving for s^*,

$$s^* = \frac{1}{b-a}\left[B - A - \frac{(b-a)^2}{2}f(a,A) + \cdots\right]$$

we see that since our approximate slope s satisfies

$$s \equiv s(\bar{a}) = \frac{1}{b-a}\left[B - A - \frac{(b-a)^2}{2}f(a,A) - \frac{h^3}{6}\sum_{i=1}^{n} c_i^n a_i\right],$$

taking $\bar{a}^{(0)} = \bar{0}$ results in using

$$s^{(0)} \equiv s(\bar{a}^{(0)}) = s(\bar{0}) = \frac{1}{b-a}\left[B - A - \frac{(b-a)^2}{2}f(a,A)\right]$$

as our initial approximation to the exact slope s^*. Also note that $s^{(0)}$ is the slope at $x = a$ of the quadratic polynomial $p(x)$ passing through the points (a,A), (b,B), and satisfying $p''(a) = f(a,A)$.

III. THE CONSISTENCY RELATION FOR A SPLINE FUNCTION

In this chapter we will prove two important results which will be used in the next chapter in proving the convergence of our constructed spline function approximation to the solution of (1.1). These results are analogous to those described by Loscalzo and Talbot [8] in their treatment of the initial value problem (1.4). For completeness, we include the following discussion by Curry and Schoenberg [4] on their description of a basis for S_m which is obtained after first considering splines defined on $(-\infty,\infty)$.

Let

$$\cdots < x_{-2} < x_{-1} < x_o < x_1 < x_2 < \cdots < x_i < \cdots \qquad (3.1)$$

be a sequence of reals, such that $x_i \to \pm\infty$ as $i \to \pm\infty$, and let m be a natural number. By a spline function $S(x)$ of degree m having the knots (3.1), we mean a function of class $C^{m-1}(-\infty,\infty)$, such that in each interval (x_i,x_{i+1}) it reduces to a polynomial of degree not exceeding m. Next we define a particular example of such a spline function in terms of divided differences.

Definition 3.1: Consider the subset $\{x_o,x_1,x_2,\ldots,x_{m+1}\}$ of the set of points listed in (3.1). Let

$$u_+ = \begin{cases} u, & \text{if } u \geqq 0 \\ 0, & \text{if } u < 0 \end{cases},$$

$$\omega(x) = (x-x_o)(x-x_1)\ \ldots\ (x-x_{m+1}) \tag{3.2}$$

and

$$M(x;x_o,x_1,\ldots,x_{m+1}) = \sum_{i=0}^{m+1} \frac{(m+1)(x_i-x)_+^m}{\omega'(x_i)}\ . \tag{3.3}$$

If we think of $M(x) = M(x;x_o,x_1,\ldots,x_{m+1})$ as the divided difference of the function

$$M(x;t) = (m+1)(t-x)_+^m \tag{3.4}$$

based on the points $t = x_o,x_1,\ldots,x_{m+1}$, this notation becomes consistent with Steffensen's notation [11] for divided differences. From (3.3) it is easily apparent that $M(x) \varepsilon \pi_m$ in each of the intervals (x_{i-1},x_i), $i = 1,\ldots,m+1$, while $M(x) = 0$ if $x < x_o$ as we can remove the subscript "+" in (3.3) and the sum then vanishes as a divided difference of order $m+1$ of a polynomial of degree m. Moreover, by the definition of the function u_+, $M(x)$ clearly vanishes for $x > x_{m+1}$. We note also that $M(x) \varepsilon C^{m-1}(-\infty,\infty)$ and hence $M(x)$ is a spline function of degree m defined on the interval $(-\infty,\infty)$.

We now state the representation theorem [4,p.80]:

Theorem 3.1: Given the knots (3.1) we consider the sequence of spline functions

$$M_j(x) = M(x;x_j,x_{j+1},\ldots,x_{j+m+1}), \quad -\infty < j < \infty \tag{3.5}$$

Every spline $S(x)$ of degree m defined on $(-\infty,\infty)$ with the knots (3.1) may be uniquely represented in the form

$$S(x) = \sum_{-\infty}^{\infty} c_j M_j(x) \tag{3.6}$$

with constants c_j. Conversely, every series (3.6) with arbitrary constants c_j defines such a spline function $S(x)$.

For this reason, because they provide a basis for the class of spline functions, functions of the form (3.3), or (3.5), will be called B-splines. Observe that if we assume the knots in (3.1) are equidistant, say $x_{i+1} - x_i = h$ for all i, then by equation (3.5) we have

$$M_j(x) = M(x;x_o + jh, x_o + (j+1)h, \ldots, x_o + (j+m+1)h), \quad -\infty < j < \infty \tag{3.7}$$

It is clear from the geometry of the situation that these are translates of one and the same function $Q_{m+1}(x)$ which can be expressed in several equivalent ways in view of (3.3):

$$Q_{m+1}(x) = M_o(x) \tag{3.8}$$

$$Q_{m+1}(x) = \frac{1}{m!h^n} \sum_{i=0}^{m+1} (-1)^{m+1-i} \binom{m+1}{i} (x_o + ih - x)_+^m \tag{3.9}$$

$$Q_{m+1}(x) = \frac{1}{m!h^m} \sum_{i=0}^{m+1} (-1)^i \binom{m+1}{i} [x - (x_o + ih)]_+^m, \tag{3.10}$$

and $\quad M_j(x) = Q_{m+1}(x - jh)$. For $m = 3$, (3.11)

these functions are illustrated in the figure below.

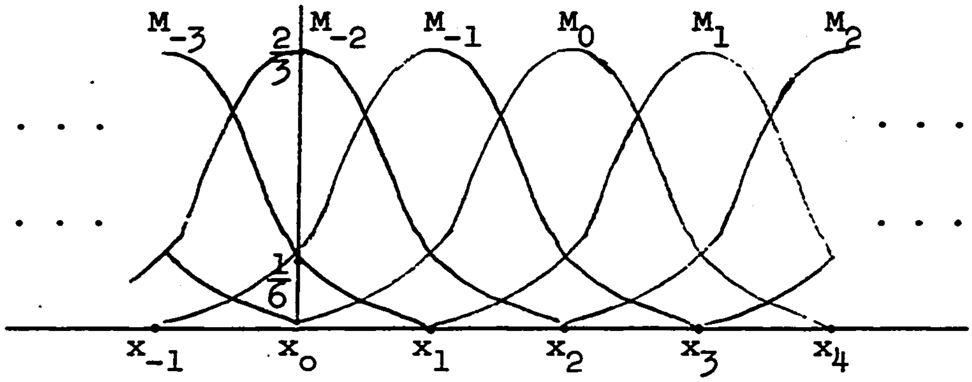

Figure 3.1

The basis functions $M_j(x)$ for $m = 3$

Returning now to the class $\mathcal{S}_m$ defined in Definition 1.2, we can determine an appropriate basis for this class. First, if $S(x) \in \mathcal{S}_m$, we define x_i to be a knot of multiplicity $r(0 \leqq r \leqq m + 1)$ if in a sufficiently small neighborhood of x_i, $S(x) \in C^{m-r}$. Thus $r = 0$ means that x_i is really not a knot. At the other extreme, $r = m + 1$ means that there are no continuity requirements between the two components of the spline function, below and above x_i. Recall now that $S(x) \in \mathcal{S}_m$ was defined over a finite interval $[a,b]$ containing the $n - 1$ knots, x_i, $i = 1,2,\ldots,n-1$, satisfying

$$a < x_1 < x_2 < \cdots < x_{n-1} < b. \tag{3.12}$$

We now introduce two more knots

$$x_o = a,\ x_n = b, \quad \text{both of multiplicity} \quad m + 1. \tag{3.13}$$

Hence we really have now $2(m+1) + n - 1$ knots, a fact which we indicate by writing out the knots as follows:

$$\overbrace{x_o, x_o, \ldots, x_o}^{m+1}, x_1, x_2, \ldots, x_{n-1}, \overbrace{x_n, x_n, \ldots, x_n}^{m+1}. \tag{3.14}$$

A basis for the family S_m is now formed by the following $m + n$ B-splines

$$\begin{aligned}
M_o(x) &= M(x;\overbrace{x_o, \ldots, x_o}^{m+1}, x_1), \\
M_1(x) &= M(x;\overbrace{x_o, \ldots, x_o}^{m}, x_1, x_2), \\
&\ \ \vdots \\
M_\ell(x) &= M(x;x_{n-1}, \overbrace{x_n, x_n, \ldots, x_n}^{m+1}),
\end{aligned} \tag{3.15}$$

where we set

$$\ell = m + n - 1 \tag{3.16}$$

Observe, however, that equation (3.3) is no longer valid for multiple knots and must be replaced by the appropriate expressions for confluent divided differences.

Now let $\mathcal{S} \subset \mathcal{S}_m$ denote the class of spline functions with knots $x_i = a + ih$, $i = 1,\dots,n-1$. Let $S(x) \in \mathcal{S}$. If restricted to the interval $[a, a+(m-1)h]$, $S(x)$ depends on $(m+1) + (m-2) = 2m - 1$ linear parameters. It follows that the $2m$ quantities

$$S(a+ih),\ S''(a+ih),\ i = 0,1,\dots,m-1 \tag{3.17}$$

cannot be linearly independent. In fact we have the following:

<u>Theorem 3.2</u>: For any spline function $S(x) \in \mathcal{S}$, there is a unique linear relation between the quantities (3.17) given by

$$\sum_{i=0}^{m-1} \alpha_i^{(m)} S(a+ih) = h^2 \sum_{i=0}^{m-1} \beta_i^{(m)} S''(a+ih) \tag{3.18}$$

whose coefficients may be written as

$$\alpha_i^{(m)} = (m-2)!\,[Q_{m-1}(i+1) - 2Q_{m-1}(i) + Q_{m-1}(i-1)] \tag{3.19}$$

$$\beta_i^{(m)} = (m-2)!Q_{m+1}(i+1) \tag{3.20}$$

where $$Q_{m+1}(x) = \frac{1}{m!}\sum_{i=0}^{m+1} (-1)^i \binom{m+1}{i}(x-i)_+^m \tag{3.21}$$

which is a B-spline.

Proof: This is a mild extension of the proof of Theorem 2.2 appearing in [8] which was due to Schoenberg.

We first make the change of scale $z = \frac{n}{b-a}(x-a)$ so that without loss of generality we may take $h = 1$ and $a = 0$ in equation (3.18). Next, consider the convolution of two infinite sequences defined by

$$\{a_n\} * \{b_n\} = \{c_n\}$$

where

$$c_n = \sum_k a_k b_{n-k}, \quad -\infty < n < \infty.$$

The following properties hold for convolution:

$$\begin{aligned} \{a_n\} * \{b_n\} &= \{b_n\} * \{a_n\} \\ \{a_n\} * \{b_n\} &= \{a_{n-i}\} * \{b_{n+i}\} \end{aligned} \tag{3.22}$$

We now consider the B-spline $Q(x) = Q_{m+1}(x)$ defined by (3.21) and examine the convolution of $\{Q''(n)\}$ with $\{Q(n-i)\}$. Applying relations (3.22), we have

$$\begin{aligned}\{Q''(n)\} * \{Q(n-i)\} &= \{Q(n-i)\} * \{Q''(n)\} \\ &= \{Q(n)\} * \{Q''(n-i)\}\end{aligned} \tag{3.23}$$

If we apply the representation Theorem 3.1 we may write the arbitrary spline function $S(x)$ as

$$S(x) = \sum_i c_i Q(x-i).$$

In particular we have

$$\begin{aligned}S(n) &= \sum_i c_i Q(n-i) \\ S''(n) &= \sum_i c_i Q''(n-i).\end{aligned} \tag{3.24}$$

Combining relations (3.23) and (3.24) finally yields

$$\{Q''(n)\} * \{S(n)\} = \{Q(n)\} * \{S''(n)\}. \tag{3.25}$$

We observe from (3.21) that $Q(x) = Q_{m+1}(x)$ vanishes outside the interval $(0, m+1)$. Taking the element $n = m$ of the convolution on each side of equation (3.25) now yields a result in the form of (3.18) with coefficients

$$\alpha_i^{(m)} = Q''_{m+1}(m-i), \quad \beta_i^{(m)} = Q_{m+1}(m-i). \tag{3.26}$$

But the coefficients defined in (3.19)-(3.20) differ from these only by a constant factor of $(m-2)!$ because B splines have the symmetry properties

$$Q_{m+1}(m-x) = Q_{m+1}(x+1)$$

$$Q'_{m+1}(m-x) = -Q'_{m+1}(x+1)$$

$$Q''_{m+1}(m-x) = Q''_{m+1}(x+1)$$

and the differentiation properties

$$Q'_{m+1}(x+1) = Q_m(x+1) - Q_m(x)$$

$$Q''_{m+1}(x+1) = Q_{m-1}(x+1) - 2Q_{m-1}(x) + Q_{m-1}(x-1).$$

These relations can be verified directly from (3.21), and this completes the proof.

For $m = 3,4,5$ the coefficients of the consistency relation (3.18) are given in the following table.

Table 3.1

Coefficients of the consistency relations

m\i	0	1	2	3	4	0	1	2	3	4
3	1	-2	1			$\frac{1}{6}$	$\frac{4}{6}$	$\frac{1}{6}$		
4	1	-1	-1	1		$\frac{1}{12}$	$\frac{11}{12}$	$\frac{11}{12}$	$\frac{1}{12}$	
5	1	2	-6	2	1	$\frac{1}{20}$	$\frac{26}{20}$	$\frac{66}{20}$	$\frac{26}{20}$	$\frac{1}{20}$

We now prove the second result which exhibits the relation between the values of the cubic spline function constructed in Chapter II and those of a certain multistep method at the points $x_i = a + ih$, $i = 0,1,\ldots,n$.

Theorem 3.3: Assume that $h < \sqrt{\frac{6}{L}}$ where L is the Lipschitz constant for f. Then the values $S(a+ih,s)$, $i = 0,1,\ldots,n$ obtained in Chapter II are precisely the values furnished by the discrete multistep method described by the recurrence relation

$$\sum_{i=0}^{2} \alpha_i^{(3)} y_{k-2+i} = h^2 \sum_{i=0}^{2} \beta_i^{(3)} y''_{k-2+i}, \quad k = 2,\ldots,n \qquad (3.27)$$

or

$$y_k - 2y_{k-1} + y_{k-2} = \frac{h^2}{6}[f_k + 4f_{k-1} + f_{k-2}], \qquad k = 2,\ldots,n \tag{3.28}$$

if the starting values

$$y_o = S(a,s) \quad \text{and} \quad y_1 = S(a+h,s) \tag{3.29}$$

are used.

<u>Proof</u>: For $h < \sqrt{\frac{6}{L}}$ only one sequence $\{y_i\}$, $i = 2,\ldots,n$ satisfies (3.27) with starting values (3.29). By the consistency relation (3.18), however, the sequence $\{S(a+ih,s)\}$ satisfies (3.27) and obviously has starting values (3.29). Thus the values $S(a+ih,s)$, $i = 2,\ldots,n$, must coincide with the points y_i generated by the multi-step method.

IV. CONVERGENCE PROPERTIES

In Chapter III we found that the cubic spline function constructed in Chapter II furnished the same discrete solution $S(a+kh,s)$, $k = 0,1,\ldots,n$, as the 2-step method

$$y_k - 2y_{k-1} + y_{k-2} = \frac{h^2}{6}[f_k + 4f_{k-1} + f_{k-2}] \tag{4.1}$$

provided that $y_o = S(a,s)$ and $y_1 = S(a+k,s)$ are used as starting values. Except where appropriate, we will now delete for notational convenience the dependence on the parameter s by writing $S(x)$ in place of $S(x,s)$.

For $S(x) \in \mathcal{S}_m$ we now define the step function $S^{(m)}(x)$ at the knots $x_k = a+kh$, $k = 1,\ldots,n-1$, by the usual arithmetic mean:

$$S^{(m)}(x_k) = \frac{1}{2}\left[S^{(m)}\left(x_k - \frac{h}{2}\right) + S^{(m)}\left(x_k + \frac{h}{2}\right)\right] \qquad k = 1,\ldots,n-1. \tag{4.2}$$

We then have the following theorem which exhibits how closely the constructed spline function approximates the solution $y(x,s)$ of the initial value problem (2.3)-(2.4).

<u>Theorem 4.1</u>: If $f(x,y) \in C^2$ in T, then there exists a constant K such that for all $h < \sqrt{\frac{6}{L}}$,

$$|y(x,s) - S(x)| < Kh^2, \quad |y'(x,s) - S'(x)| < Kh^2,$$

$$|y''(x,s) - S''(x)| < Kh^2, \quad |y'''(x,s) - S'''(x)| < Kh,$$

if $x \in [a,b]$, provided $S'''(x_k)$ is given by (4.2) with $m = 3$.

The proof of this convergence theorem depends on some lemmas. First we note that the multistep method defined by (4.1) is of second order accuracy provided the starting values have third order accuracy [6,p.314]. We therefore begin by considering the error in the starting value $y_1 = S(a+h,s)$ noting that by construction $y_o = S(a,s) = y(a,s) = A$.

<u>Lemma 4.2</u>: If f_x and f_y are bounded in T and $|y'(x,s)| \leqq Q$ for $x \in [a,b]$, then there exists a constant K such that

$$|y(a+h,s) - S(a+h,s)| < Kh^3.$$

<u>Proof</u>: Consider the expressions

$$y(a+h,s) = y(a,s) + hy'(a,s) + \frac{h^2}{2} y''(a,s) + \frac{h^3}{6} y'''(\xi,s),$$

$$a < \xi < a + h,$$

$$S(a+h,s) = y(a,s) + hy'(a,s) + \frac{h^2}{2} y''(a,s) + \frac{h^3}{6} a_1.$$

Thus we have

$$|y(a+h,s) - S(a+h,s)| = \frac{h^3}{6}|y'''(\xi,s) - a_1|.$$

But since

$$y'''(\xi,s) = f_x(\xi,y(\xi,s)) + f_y(\xi,y(\xi,s))y'(\xi,s),$$

$$|y'''(\xi,s) - a_1| \leq |f_x(\xi,y(\xi,s))| + |f_y(\xi,y(\xi,s))||y'(\xi,s)| + |a_1|.$$

Letting $M_1 = \max\limits_{(x,y)\epsilon T} |f_x(x,y)|$, $M_2 = \max\limits_{(x,y)\epsilon T} |f_y(x,y)|$, we get

$$|y'''(\xi,s) - a_1| \leq M_1 + M_2Q + |a_1| \equiv K.$$

Hence

$$y(a+h,s) - S(a+h,s) \doteq O(h^3).$$

Lemma 4.3: If $|y(x_k,s) - S(x_k)| < Kh^p$ and $S''(x_k) = f(x_k,S(x_k))$, then there exists a constant K^* such that

$$|y(x_k,s) - S(x_k)| < K^*h^p \quad \text{and} \quad |y''(x_k,s) - S''(x_k)| < K^*h^p.$$

Proof: This is an immediate consequence of the Lipschitz condition. We have explicitly

$$|y''(x_k,s) - S''(x_k)| = |f(x_k,y(x_k,s)) - f(x_k,S(x_k))|$$

$$\leq L|y(x_k,s) - S(x_k)| < LKh^p.$$

Simply let $K^* = \max\{K, LK\}$.

The next result is due to Loscalzo and Talbot [8].

Lemma 4.4: Let $y(x,s) \in C^{m+1}[a,b]$ and let $S(x)$ be a spline function of degree m having its knots at the points x_k, $k = 1,2,\ldots,n-1$, and such that the conditions

$$|y^{(r)}(x_k,s) - S^{(r)}(x_k)| = O(h^{p_r}),\quad r = 0,1,\ldots,m-1;$$
$$k = 0,1,\ldots,n-1, \tag{4.3}$$

$$|y^{(m)}(x,s) - S^{(m)}(x)| = O(h),\quad x_k < x < x_{k+1};$$
$$k = 0,1,\ldots,n-1, \tag{4.4}$$

are satisfied. Then,

$$|y(x,s) - S(x)| = O(h^p),\quad x \in [a,b] \tag{4.5}$$

where
$$p = \min_{r=0,1,\ldots,m} (r + p_r) \tag{4.6}$$

where $p_m = 1$ and furthermore

$$|y^{(m)}(x,s) - S^{(m)}(x)| = O(h),\quad x \in [a,b]. \tag{4.7}$$

<u>Proof</u>: Let $x_k < x \leqq x_{k+1}$. Expanding by Taylor's theorem and writing $\omega = x - x_k \leqq h$, we obtain

$$y(x,s) = \sum_{r=0}^{m-1} \frac{1}{r!} \omega^r y^{(r)}(x_k,s) + \frac{1}{m!} \omega^m y^{(m)}(\xi,s), \qquad (4.8)$$

$$x_k < \xi < x,$$

$$s(x) = \sum_{r=0}^{m-1} \frac{1}{r!} \omega^r s^{(r)}(x_k) + \frac{1}{m!} \omega^m s^{(m)}(\xi). \qquad (4.9)$$

Note that $s^{(m)}(x)$ is constant for $x_k < x < x_{k+1}$. Subtraction of (4.9) from (4.8) gives

$$|y(x,s) - s(x)| \le \sum_{r=0}^{m-1} \frac{1}{r!} h^r |y^{(r)}(x_k,s) - s^{(r)}(x_k)|$$

$$+ \frac{1}{m!} h^m |y^{(m)}(\xi,s) - s^{(m)}(\xi)| = O(h^p)$$

in view of (4.3), (4.4), and (4.6). This establishes (4.5). To prove (4.7) it is sufficient, in view of (4.4), to consider the knots x_k, $k = 1,2,\ldots,n-1$. By (4.2) and (4.4),

$$s^{(m)}(x_k) = \frac{1}{2}\left[s^{(m)}\left(x_k - \frac{h}{2}\right) + s^{(m)}\left(x_k + \frac{h}{2}\right)\right]$$

$$= \frac{1}{2}\left[y^{(m)}\left(x_k - \frac{h}{2}, s\right) + y^{(m)}\left(x_k + \frac{h}{2}, s\right)\right] + O(h).$$

But, since $y(x,s) \in C^{m+1}[a,b]$,

$$y^{(m)}\left(x_k - \frac{h}{2}, s\right) = y^{(m)}(x_k, s) - \frac{1}{2} h y^{(m+1)}(\xi_1, s),$$

$$x_k - \frac{h}{2} < \xi_1 < x_k,$$

$$y^{(m)}\left(x_k + \frac{h}{2}, s\right) = y^{(m)}(x_k, s) + \frac{1}{2} h y^{(m+1)}(\xi_2, s),$$

$$x_k < \xi_2 < x_k + \frac{h}{2}.$$

Thus we finally obtain

$$s^{(m)}(x_k) = y^{(m)}(x_k, s) + 0(h), \quad K = 1,2,\ldots,n-1.$$

This completes the proof.

Lemma 4.5: If $|y''(x,s) - s''(x)| < Kh^p$ for $x \in [a,b]$, then there exists a constant K_o such that

$$|y'(x,s) - S'(x)| < K_o h^p, \tag{4.10}$$

and in particular this holds at the points x_k, $k = 0,1,\ldots,n-1$.

<u>Proof</u>: We note that

$$y'(x,s) - S'(x) = \int_a^x [y''(t,s) - S''(t)]dt,$$

and hence

$$|y'(x,s) - S'(x)| \leq \int_a^x |y''(t,s) - S''(t)|dt$$

$$< (x - a)Kh^p \leq (b - a)Kh^p.$$

Simply let $K_o = (b - a)K$.

<u>Proof of Theorem 4.1</u>: Let $m = 3$. We have shown that the cubic spline values $S_k = S(x_k)$ are the same as the values generated by the multistep method (4.1) which is a second order method provided the starting values have third order accuracy. The latter we have shown to be true in Lemma 4.2. Therefore there exists a constant K_1 such that

$$|y_k - S_k| < K_1h^2, \ k = 0,1,\ldots,n$$

and

$$|y_k'' - S_k''| < K_1h^2, \ k = 0,1,\ldots,n$$

by Lemma 4.3. Expanding $y''_{k+1} = y''(x_{k+1}, s)$ and $S''_{k+1} = S'(x_{k+1})$ by Taylor's theorem gives

$$y''_{k+1} = y''_k + hy'''(\xi, s), \quad x_k < \xi < x_{k+1}$$

$$S''_{k+1} = S''_k + hS'''(x),$$

for any $x \in (x_k, x_{k+1})$. Therefore,

$$h|y'''(\xi,s) - S'''(x)| \leq |y''_k - S''_k| + |y''_{k+1} - S''_{k+1}|,$$

and hence

$$S'''(x) = y'''(\xi, s) + O(h),$$

which because $|\xi - x| < h$, we may write as

$$S'''(x) = y'''(x, s) + O(h).$$

Now the hypothesis of Lemma 4.4 are satisfied for $S''(x)$ which is a spline function of degree 1 with the same knots as $S(x)$. Hence letting $S''(x)$ assume the role of $S(x)$ in that Lemma we find

$$|y''(x,s) - S''(x)| = 0(h^2),\ x \in [a,b],$$

which establishes the third inequality in Theorem 4.1. Next by Lemma 4.5,

$$|y'(x_k,s) - S'(x_k)| = 0(h^2)$$

and finally by applying Lemma 4.4 twice, allowing $S(x)$ and $S'(x)$, successively, to assume the role of $S(x)$ in the Lemma establishes the first two inequalities of Theorem 4.1. The fourth inequality follows from equation (4.7), since $f \in C^2$ in T implies $y(x) \in C^4[a,b]$ as required by the hypothesis of Lemma 4.4.

Finally, we are concerned with how closely $S(x,s)$ approximates the solution $y(x)$ of the boundary value problem (1.1) or, equivalently, the solution $y(x,s^*)$ of the initial value problem

$$y'' = f(x,y),\ y(a) = A,\ y'(a) = s^*. \tag{4.11}$$

Recall that $y(x,s)$ is the solution of the initial value problem

$$y'' = f(x,y),\ y(a) = A,\ y'(a) = s,$$

where s is the initial slope determined by the equation $S(b,s) = B$, rather than $y(b,s) = B$. Hence we will let

$$y(b,s) = \tilde{B}. \tag{4.12}$$

Of course $\tilde{B} \neq B$ in general but since $S(b,s) = B$,

$$|B - \tilde{B}| = |S(b,s) - y(b,s)| = O(h^2) \tag{4.13}$$

by Theorem 4.1. Next, consider the following concept discussed in a more general context in a paper by Gaines [5]:

<u>Definition 4.1</u>: Solutions to $y'' = f(x,y)$ will be said to satisfy the maximum principle on $[a,b]$ if for any solutions $\varphi(x)$ and $\psi(x)$, $|\varphi(x) - \psi(x)|$ assumes its maximum on $[a,b]$ at either a or b.

Various sets of hypothesis on $f(x,y)$ imply that solutions to $y'' = f(x,y)$ satisfy the maximum principle on $[a,b]$. One such set is that $f(x,y)$ be continuous on T, and $f(x,y)$ be nondecreasing in y on T. Hence we see that for the type of problems under consideration, namely those of class M, the maximum principle applies.

Consider now the difference

$$|y(x,s^*) - S(x,s)| \leq |y(x,s^*) - y(x,s)| + |y(x,s) - S(x,s)|, \tag{4.14}$$

but

$$|y(x,s^*) - y(x,s)| \leq \max\{|A - A|, |B - \tilde{B}|\} = |B - \tilde{B}| = O(h^2)$$

by the maximum principle and equation (4.13). Also,

$$|y(x,s) - S(x,s)| = O(h^2)$$

by Theorem 4.1. Hence from (4.14) we see that

$$|y(x,s^*) - S(x,s)| < c_1 h^2, \quad x \in [a,b]. \tag{4.15}$$

Similarly,

$$|y''(x,s^*) - S''(x,s)| \leq |y''(x,s^*) - y''(x,s)| + |y''(x,s) - S''(x,s)|. \tag{4.16}$$

But

$$|y''(x,s^*) - y''(x,s)| = |f(x,y(x,s^*)) - f(x,y(x,s))|$$

$$\leqq L|y(x,s^*) - y(x,s)| < c_1 L h^2$$

and $|y''(x,s) - S''(x,s)| = 0(h^2)$ by Theorem 4.1. Hence from (4.16) we have

$$|y''(x,s^*) - S''(x,s)| < c_2 h^2, \ x \in [a,b]. \tag{4.17}$$

Also,

$$|y'(x,s^*) - S'(x,s)| \leqq |y'(x,s^*) - y'(x,s)| + |y'(x,s) - S'(x,s)|, \tag{4.18}$$

and since

$$|y'(x,s^*) - y'(x,s)| \leqq \int_a^x |y''(t,s^*) - y''(t,s)|dt$$

$$< (x-a)c_2 h^2 \leqq (b-a)c_2 h^2$$

and

$$|y'(x,s) - S'(x,s)| = 0(h^2)$$

from Theorem 4.1, we get

$$|y'(x,s^*) - S'(x,s)| < C_3h^2, \ x \in [a,b]. \tag{4.19}$$

Since by Theorem 4.1,

$$|y'''(x,s) - S'''(x,s)| < Kh$$

we suggest that it may be possible to show that

$$|y'''(x,s^*) - S'''(x,s)| < C_4h$$

for some constant C_4.

V. EXAMPLES

Several examples using the cubic spline approximation were programmed on the IBM 360/65 computer, some of which are listed on the following pages. The results illustrate the $O(h^2)$ accuracy which was calculated according to the following formulation:

Given two different integers n_j, $j = 1,2$, we let $h_j = (b-a)/n_j$ and $\varepsilon_j = \max_{0 \leq i \leq n_j} |S_i - y_i|$, where $S_i \equiv S(x_i,s)$ and $y_i = y(x_i,s^*)$ are the values of the spline approximation and the exact solution respectively at the points $x_i = a + ih_j$, $i = 0,1,\ldots,n_j$, $j = 1,2$. Then

$$\varepsilon_j = Kh_j^{\alpha},\ j = 1,2, \tag{5.1}$$

for some α and proportionality constant K. Hence the parameter α from equations (5.1) is given by

$$\alpha = -\frac{\ln \varepsilon_1 - \ln \varepsilon_2}{\ln n_1 - \ln n_2}\ . \tag{5.2}$$

Similarly, we have calculated the orders of accuracy α' and α'' in approximating the first and second derivatives respectively of the exact solution by the cubic spline function at the points $x_i = a + ih_j$, $i = 0,1,\ldots,n$, $j = 1,2$.

The first example

$$y'' = (1+x^2)y, \quad y(-1) = y(1) = 1,$$

has the unique solution

$$y(x) = e^{\frac{1}{2}(x^2-1)}.$$

A Lipschitz constant for $f(x,y) = (1+x^2)y$ is $L = 2$. The boundary value problem

$$y'' = e^y, \quad y(0) = y(1) = 0,$$

considered in the second example, has the unique solution

$$y(x) = -\ln 2 + 2\ln\left[c \sec\left\{c(x-\tfrac{1}{2})/2\right\}\right]$$

where c is the root of $\sqrt{2} = c\sec\left(\frac{c}{4}\right)$ which lies between 0 and $\frac{\pi}{2}$, namely, $c = 1.3360557$ to eight figures. The third example

$$y'' = \tfrac{1}{2}(y+x+1)^3, \quad y(0) = y(1) = 0$$

possesses the unique solution

$$y(x) = \frac{2}{2-x} - x - 1.$$

Examples two and three appear in [2,p.425].

The last example

$$y'' = \frac{3}{2}y^2,\ y(0) = 4,\ y(1) = 1$$

has two solutions [3,p.145], one of which is

$$y(x) = \frac{4}{(1+x)^2},$$

and the other is in terms of elliptic functions.

Observe that the functions $f(x,y)$ is examples two and three above possess a unique solution but do not satisfy a Lipschitz condition for all y as is also true for many other functions. However, in considering those functions $f(x,y)$ for which $f_y(x,y) \geqq 0$ in T, we may apply the bound:

$$|y(x)| \leqq \frac{(b-a)^2}{8} M$$

where M is a constant such that

$$M > |f(x,0)|, \ x \in [a,b].$$

This is described by Bailey, Shampine, and Waltman [1, p.116]. Hence the Lipschitz constant L can be taken as

$$L = \max|f_y(x,y)|, \ x \in [a,b], \ |y| \leq \frac{(b-a)^2}{8} M.$$

In example two with $f(x,y) = e^y$, we then can take $L = e^{1/8}$ and for $f(x,y) = \frac{1}{2}(y+x+1)^3$, as in example three, $L = 75/8$.

Example four as pointed out above, does not possess a unique solution and was included to see whether or not the method would converge to one of the solutions.

As mentioned previously, examples two and three are discussed by Ciarlet, Schultz, and Varga in [2] wherein numerical methods are developed for solving the more general two-point boundary value problem:

$$L[y(x)] = f(x,y(x)), \ 0 < x < 1 \tag{5.3}$$

$$D^k u(0) = D^k u(1) = 0, \ D = \frac{d}{dx}, \ 0 \leq k \leq n-1, \tag{5.4}$$

where the linear differential operator L is defined by

$$L[y(x)] = \sum_{j=o}^{n} (-1)^{j+1} D^j [p_j(x) D^j y(x)], \; n \geqq 1.$$

The boundary conditions $D^k u(a) = A$, $D^k u(b) = B$ can be reduced to the case $a = 0$, $b = 1$, $A = B = 0$ by means of a suitable change of the independent and dependent variables. Our problem (1.1) then results by taking $n = 1$, $p_o(x) \equiv 0$, and $p_1(x) \equiv 1$.

Their approach to the problem is in applying the Rayleigh-Ritz procedure to the variational formulation of (5.3)-(5.4) by minimizing over subspaces of polynomial functions, and piecewise-polynomial functions such as Hermite and spline functions. In particular, for cubic spline functions, $0(h^2)$ convergence to the solution $y(x)$ of (5.3)-(5.4) is established but in a quite different fashion then described here. In following the construction of the approximating function as described by Ciarlet, Schultz, and Varga [2, p.397-399], we note that it is also necessary to solve a nonlinear system of the form:

$$A\bar{u} + \bar{g}(\bar{u}) = \bar{0}.$$

Here $A = (a_{i,k})$ is a $M \times M$ real matrix, and $\bar{g}(\bar{u}) = (g_1(\bar{u}),\ldots,g_n(\bar{u}))^T$ is a column vector, being determined respectively by

$$a_{i,k} = \int_o^1 \left\{ \sum_{j=o}^{n} p_j(x) D^j \omega_i(x) D^j \omega_k(x) \right\} dx, \quad 1 \leqq i,k \leqq M, \tag{5.5}$$

and

$$g_k(\bar{u}) = \int_o^1 f(x, \sum_{i=1}^{M} u_i \omega_i(x)) \omega_k(x) dx, \quad 1 \leqq k \leqq M, \tag{5.6}$$

where M is the dimension of the subspace and $\{\omega_i(x)\}_{i=1}^{M}$ are M linearly independent functions from the subspace.

The approach we take also results in solving the non-linear system of equations (2.21) arising from the collocation requirements, however, it is far simpler computationally as it avoids evaluations of the various integrals as in (5.6).

Example 1: $y'' = (1+x^2)y,\ y(-1) = y(1) = 1$

Results: $n = 16 \quad h = 0.1250000$

X	S(X)	Y(X)	S'(X)	Y'(X)	S''(X)	Y''(X)
-1.0000000	1.0000000	1.0000000	-1.0041010	-1.0000000	2.0000000	2.0000000
-0.8750000	0.8889915	0.8894184	-0.7810003	-0.7782410	1.5696230	1.5703790
-0.7500000	0.8028083	0.8035225	-0.6044997	-0.6026419	1.2543850	1.2555030
-0.6250000	0.7364461	0.7373537	-0.4620932	-0.4608461	1.0241170	1.0253820
-0.5000000	0.6862522	0.6872892	-0.3444726	-0.3436446	0.8578128	0.8591115
-0.3750000	0.6495904	0.6507124	-0.2445509	-0.2440171	0.7409363	0.7422188
-0.2500000	0.6246088	0.6257840	-0.1567646	-0.1564460	0.6636441	0.6648955
-0.1250000	0.6100833	0.6112877	-0.0765611	-0.0764109	0.6196129	0.6208391
0.0000000	0.6053166	0.6065306	-0.0000032	0.0000000	0.6053138	0.6065306
0.1250000	0.6100824	0.6112877	0.0765546	0.0764109	0.6196121	0.6208391
0.2500000	0.6246071	0.6257840	0.1567580	0.1564460	0.6636422	0.6648955
0.3750000	0.6495878	0.6507124	0.2445439	0.2440171	0.7409333	0.7422188
0.5000000	0.6862487	0.6872892	0.3444652	0.3436446	0.8578081	0.8591115
0.6250000	0.7364415	0.7373537	0.4620851	0.4608461	1.0241100	1.0253820
0.7500000	0.8028026	0.8035225	0.6044905	0.6026419	1.2543760	1.2555030
0.8750000	0.8889846	0.8894184	0.7809898	0.7782410	1.5696110	1.5703790
1.0000000	0.9999917	1.0000000	1.0040890	1.0000000	1.9999810	2.0000000

Errors: $n = 16 \quad h = 0.1250000$

$\epsilon = 0.0012140 \qquad \epsilon' = 0.0041018 \qquad \epsilon'' = 0.0013034$

Errors: $n = 64 \quad h = 0.0312500$

$\epsilon = 0.0000787 \qquad \epsilon' = 0.0002584 \qquad \epsilon'' = 0.0000883$

Calculated Order of Accuracy:

$\alpha = 1.9738460 \qquad \alpha' = 1.9941530 \qquad \alpha'' = 1.9416000$

Example 2: $y'' = e^y$, $y(0) = y(1) = 0$

Result: n = 16 h = 0.0625000

X	S(X)	Y(X)	S'(X)	Y'(X)	S''(X)	Y''(X)
0.0000000	0.0000000	-0.0000005	-0.4637734	-0.4636325	1.0000000	0.9999995
0.0625000	-0.0270501	-0.0270433	-0.4021074	-0.4019898	0.9733123	0.9733191
0.1250000	-0.0502954	-0.0502810	-0.3419743	-0.3418774	0.9509482	0.9509621
0.1875000	-0.0698234	-0.0698035	-0.2831147	-0.2830368	0.9325581	0.9325770
0.2500000	-0.0857062	-0.0856829	-0.2252890	-0.2252284	0.9178633	0.9178852
0.3125000	-0.0980013	-0.0979750	-0.1682730	-0.1682285	0.9066470	0.9066716
0.3750000	-0.1067527	-0.1067234	-0.1118544	-0.1118252	0.8987472	0.8987743
0.4375000	-0.1119913	-0.1119612	-0.0558295	-0.0558151	0.8940513	0.8940789
0.5000000	-0.1137354	-0.1137050	0.0000000	0.0000000	0.8924933	0.8925212
0.5625000	-0.1119912	-0.1119612	0.0558296	0.0558151	0.8940514	0.8940789
0.6250000	-0.1067526	-0.1067234	0.1118545	0.1118252	0.8987473	0.8987743
0.6875000	-0.0980011	-0.0979750	0.1682730	0.1682285	0.9066472	0.9066716
0.7500000	-0.0857059	-0.0856829	0.2252890	0.2252284	0.9178635	0.9178852
0.8125000	-0.0698231	-0.0698035	0.2831146	0.2830368	0.9325583	0.9325770
0.8750000	-0.0502950	-0.0502810	0.3419742	0.3418774	0.9509485	0.9509621
0.9375000	-0.0270498	-0.0270433	0.4021074	0.4019898	0.9733126	0.9733191
1.0000000	0.0000003	-0.0000005	0.4637734	0.4636325	1.0000000	0.9999995

Errors: n = 16 0.0625000

$\epsilon = 0.0000305$ $\epsilon' = 0.0001409$ $\epsilon'' = 0.0000279$

Errors: n = 64 h = 0.0156250

$\epsilon = 0.0000025$ $\epsilon' = 0.0000089$ $\epsilon'' = 0.0000024$

Calculated Order of Accuracy:

$\alpha = 1.8132450$ $\alpha' = 1.9939220$ $\alpha'' = 1.7564050$

Example 3: $y'' = \frac{1}{2}(y+x+1)^3, \; y(0) = y(1) = 0$

Result: $n = 16 \quad h = 0.0625000$

X	S(X)	Y(X)	S'(X)	Y'(X)	S''(X)	Y''(X)
0.0000000	0.0000000	0.0000000	-0.5006774	-0.5000000	0.5000000	0.5000000
0.0625000	-0.0302833	-0.0302420	-0.4678681	-0.4672217	0.5498972	0.5499644
0.1250000	-0.0584141	-0.0583334	-0.4317252	-0.4311112	0.6066747	0.6068144
0.1875000	-0.0841697	-0.0840521	-0.3917804	-0.3912010	0.6715598	0.6717772
0.2500000	-0.1072958	-0.1071434	-0.3474800	-0.3469388	0.7460518	0.7463546
0.3125000	-0.1275002	-0.1273155	-0.2981659	-0.2976680	0.8319979	0.8323917
0.3750000	-0.1444456	-0.1442308	-0.2430508	-0.2426036	0.9316859	0.9321799
0.4375000	-0.1577408	-0.1575003	-0.1811863	-0.1808000	1.0479770	1.0485740
0.5000000	-0.1669292	-0.1666670	-0.1114221	-0.1111112	1.1844760	1.1851830
0.5625000	-0.1714746	-0.1711960	-0.0323517	-0.0321361	1.3457740	1.3465910
0.6250000	-0.1707431	-0.1704550	0.0577590	0.0578508	1.5377680	1.5386900
0.6875000	-0.1639797	-0.1636906	0.1610681	0.1609974	1.7681220	1.7691380
0.7500000	-0.1502780	-0.1500006	0.2802882	0.2799997	2.0469200	2.0479970
0.8125000	-0.1285403	-0.1282902	0.4188672	0.4182825	2.3876070	2.3886830
0.8750000	-0.0974239	-0.0972223	0.5812413	0.5802460	2.8083630	2.8093270
0.9375000	-0.0552689	-0.0551472	0.7731954	0.7716255	3.3341710	3.3348240
1.0000000	0.0000014	0.0000000	1.0023880	1.0000000	4.0000050	4.0000000

Errors: $n = 16 \quad h = 0.0625000$

$\varepsilon = 0.0002891 \qquad \varepsilon' = 0.0015699 \qquad \varepsilon'' = 0.0010767$

Errors: $n = 64 \quad h = 0.0156250$

$\varepsilon = 0.0000163 \qquad \varepsilon' = 0.0001394 \qquad \varepsilon'' = 0.0000620$

Calculated Order of Accuracy:

$\alpha = 2.0756540 \qquad \alpha' = 1.7466170 \qquad \alpha'' = 2.0592300$

Example 4: $y'' = \frac{3}{2} y^2$, $y(0) = 4$, $y(1) = 1$

Result: n = 16 h = 0.0625000

X	S(X)	Y(X)	S'(X)	Y'(X)	S''(X)	Y''(X)
0.0000000	4.0000000	4.0000000	-8.0189110	-8.0000000	24.0000000	24.0000000
0.0625000	3.5423210	3.5432510	-6.6807240	-6.6696500	18.8219900	18.8319300
0.1250000	3.1590290	3.1604920	-5.6247520	-5.6186530	14.9690800	14.9830700
0.1875000	2.8348200	2.8365650	-4.7802760	-4.7773720	12.0541600	12.0691500
0.2500000	2.5581380	2.5599990	-4.0968350	-4.0959980	9.8159480	9.8303960
0.3125000	2.3201230	2.3219940	-3.5377640	-3.5382770	8.0742930	8.0874910
0.3750000	2.1138890	2.1157010	-3.0759840	-3.0773830	6.7026360	6.7142910
0.4375000	1.9340200	1.9357270	-2.6911990	-2.6931840	5.6105050	5.6205590
0.5000000	1.7762060	1.7777770	-2.3679880	-2.3703690	4.7322280	4.7407390
0.5625000	1.6369840	1.6383990	-2.0944970	-2.0971500	4.0194650	4.0265290
0.6250000	1.5135480	1.5147920	-1.8615090	-1.8643590	3.4361530	3.4418940
0.6875000	1.4036020	1.4046630	-1.6617830	-1.6647850	2.9550770	2.9596170
0.7500000	1.3052520	1.3061210	-1.4895780	-1.4927100	2.5554710	2.5589310
0.8125000	1.2169260	1.2175970	-1.3403020	-1.3435550	2.2213330	2.2238150
0.8750000	1.1373120	1.1377770	-1.2102530	-1.2136280	1.9402060	1.9418050
0.9375000	1.0653060	1.0655560	-1.0964240	-1.0999280	1.7023200	1.7031150
1.0000000	0.9999733	1.0000000	-0.9963536	-1.0000000	1.4999370	1.5000000

Errors: n = 16 h = 0.0625000

$\epsilon = 0.0018711$ $\epsilon' = 0.0189114$ $\epsilon'' = 0.0149860$

Errors: n = 64 h = 0.0156250

$\epsilon = 0.0001268$ $\epsilon' = 0.0011978$ $\epsilon'' = 0.0009184$

Calculated Order of Accuracy:

$\alpha = 1.9414120$ $\alpha' = 1.9903870$ $\alpha'' = 2.0141840$

VI. REMARKS

There arises from the previous chapters at least two interesting questions:

1. Can a spline of degree $m > 3$ be constructed in an analogous fashion in order to attain better than $0(h^2)$ convergence to the boundary value problem (1.1)-(1.2)?

2. Can a spline of degree m be constructed to approximate the solution of the general two point boundary value problem (1.3)-(1.4)?

Concerning the first question, if we denote by $f^{(p)}(x,y(x))$, $p = 1,2,...$ the total p^{th} derivative of $f(x,y(x))$ with respect to x, we could construct a spline function $S_m(x)$ of degree m to the solution $y(x,s)$ of (2.3) in the following manner. For $x \in [a,a+h]$,

$$S_m(x,s) = y(a,s)+y'(a,s)(x-a)+\frac{y''(a,s)}{2!}(x-a)^2+\frac{y'''(a,s)}{3!}(x-a)^3+\ldots$$

$$+\frac{1}{(m-1)!}y^{(m-1)}(a,s)(x-a)^{m-1}+\frac{1}{m!}a_1(x-a)^m, \qquad (6.1)$$

$$= A+s(x-a)+\frac{f(a,A)}{2!}(x-a)^2+\frac{1}{3!}[f_x(a,A)+f_y(a,A)s](x-a)^3+\ldots$$

$$+\frac{1}{(m-1)!}f^{(m-3)}(a,A)(x-a)^{m-1}+\frac{1}{m!}a_1(x-a)^m. \qquad (6.2)$$

Continuing in the fashion outlined in Chapter II, for $x \in [x_{j-1}, x_j]$, $j = 2,\ldots,n$, we define

$$S_m(x,s) = \sum_{k=0}^{m-1} \frac{1}{k!} S^{(k)}(x_{j-1},s)(x-x_{j-1})^k + \frac{1}{m!} a_j(x-x_j)^m, \tag{6.3}$$

and require

$$S_m''(x_j,s) = f(x_j,S(x_j,s)),\ j = 1,2,\ldots,n. \tag{6.4}$$

Equation (6.4) gives us n equations in the $n+1$ unknown $a_1,a_2,\ldots,a_n,s$. We now require that the spline function $S_m(x,s)$ satisfy the boundary condition at $x = b$:

$$S_m(b,s) = B. \tag{6.5}$$

As before, we may hope to express the initial slope s from equation (6.5) in terms of the n unknowns $a_1,a_2,\ldots,a_n$. From equation (6.2) we see that this may be possible for $m \leq 4$ but, for example, if $m = 5$ we need to consider $f''(a,A)$ which more explicitly becomes

$$f''(a,A) = f_{xx}(a,A) + 2f_{xy}(a,A)s + f_y(a,A)f(a,A)$$
$$+ f_{yy}(a,A)s^2,$$

so that the initial slope enters in a nonlinear fashion. Of course, we could employ the usual shooting technique as discussed in Chapter I wherein the exact solution $s = s^*$ of $\Phi(s) = y(b,s) - B = 0$ is approximated using some iterative scheme. For our development this means that we start with some initial estimate s_o of the exact slope s^* and construct a spline function $S_m(x,s_o)$ of degree m to the solution of the initial value problem

$$y'' = f(x,y),\ y(a) = A,\ y'(a) = s_o. \tag{6.6}$$

Next we check how "good" s_o is by computing $\theta(s) = S_m(b,s) - B$ at $s = s_o$. The slope s_o is then corrected by some iteration scheme, for example;

$$s_{i+1} = s_i + \theta(s_i),\ i = 0,1,\ldots \tag{6.7}$$

so that it is necessary to solve a sequence of initial value problems. As mentioned previously, Keller [7] has some general results concerning this procedure wherein the initial value problems are solved numerically by a discrete variable method.

We observe that in solving an initial value problem of the form

$$y'' = f(x,y),\ y(a) = A,\ y'(a) = s_\nu, \tag{6.8}$$

where s_ν is fixed, using a spline function $S_m(x,s_\nu) = S_m(x)$ of degree m generated by our construction, the coefficients a_i, $i = 1,\dots,n$ exist and are unique under fairly general assumptions. Note that they are determined by the conditions:

$$S_m''(x_j) = f(x_j, S_m(x_j)),\ j = 1,2,\dots,n. \tag{6.9}$$

Now over the interval $[x_{j-1}, x_j]$, we defined

$$S_m(x) = \sum_{k=0}^{m-1} \frac{1}{k!} S_m^{(k)}(x_{j-1})[x - x_{j-1}]^k + \frac{1}{m!} a_j [x - x_{j-1}]^m$$

$$= A_j(x) + \frac{a_j}{m!}(x - x_{j-1})^m,\ j = 1,2,\dots,n. \tag{6.10}$$

The $A_j(x)$ are uniquely determined by the spline continuity relations and solving for a_j from (6.9) we get

$$a_j = \frac{(m-2)!}{h^{m-2}}\left\{f(x_j, A_j(x) + \frac{1}{m!} a_j h^m) - A_j''(x)\right\}$$

$$= g(a_j) \qquad (6.11)$$

One Lipschitz constant for $g(t)$ is $\frac{Lh^2}{m(m-1)}$ independent of j where L is the Lipschitz constant for f. Hence for $h < \sqrt{\frac{m(m-1)}{L}}$ we have that $g(t)$ is a contraction mapping and equation (6.1) has a unique fixed point which may be found by iteration. Note that for such h, the corresponding difference equation has a unique solution.

Finally, we point out two interesting facts concerning question (1). If we consider approximating the solution of (1.1)-(1.2) using quartic spline functions $(m = 4)$ then, by consulting Table 3.1, we see that the corresponding multistep method is

$$y_{k-3} - y_{k-2} - y_{k-1} + y_k = \frac{h^2}{12}\left[f_{k-3} + 11f_{k-2} + 11f_{k-1} + f_k\right]. \qquad (6.12)$$

This is a stable fourth order method, and so we might expect to raise the order of convergence by constructing such a spline function.

We now prove the following negative result.

Theorem 6.1: The solutions $S_m(x)$ are divergent as $h \to 0$ for $m \geqq 5$.

Proof: We will show that the multistep methods given by the recurrence relation

$$\sum_{i=0}^{m-1} \alpha_i^{(m)} y_{k-m+1+i} = h^2 \sum_{i=0}^{m-1} \beta_i^{(m)} f_{k-m+1+i}, \qquad i = m-1, \ldots, n \tag{6.13}$$

are unstable and hence divergent for $m \geqq 5$. From Henrici [6,p.300] we know that the multistep method is stable only if the zeros of the "associated polynomial" $P(z)$ satisfy:

(i) modulus of no zero exceeds 1.

(ii) multiplicity of zeros of modulus 1 be a most 2.

Now

$$P(z) = \sum_{i=0}^{m-1} \alpha_i^{(m)} z^i$$

where

$$\alpha_i^{(m)} = (m-2)!\,[Q_{m-1}(i+1) - 2Q_{m-1}(i) + Q_{m-1}(i-1)]$$

and

$$Q_{m-1}(x) = \frac{1}{(m-2)!} \sum_{i=0}^{m-1} (-1)^i \binom{m-1}{i} (x-i)_+^{m-2}.$$

Hence

$$P(z) = (m-2)! [(z-1)^2 Q_{m-1}(1) + z(z-1)^2 Q_{m-1}(2) + \dots$$

$$+ z^{m-3}(z-1)^2 Q_{m-1}(m-2)]$$

$$= (m-2)! (z-1)^2 \sum_{i=1}^{m-2} Q_{m-1}(i) z^{i-1}$$

$$= (z-1)^2 \tilde{P}(z).$$

Utilizing the B-spline symmetry property

$$Q_{m-1}(m-1-x) = Q_{m-1}(x)$$

we see that the first two coefficients of $\tilde{P}(z)$ are

$$(m-2)! Q_{m-1}(m-2) = (m-2)! Q_{m-1}(1) = 1$$

and

$$(m-2)!Q_{m-1}(m-3) = (m-2)!Q_{m-1}(2) = 2^{m-2} - (m-1).$$

We thus have

$$\tilde{P}(z) = z^{m-3} + (2^{m-2} - m + 1)\;{}^{m-4} + \ldots + 1$$

$$= (z - r_3)(z - r_4) \ \ldots \ (z - r_{m-1}).$$

The sum of the zeros of $\tilde{P}(z)$ is given by

$$\sum_{i=3}^{m-1} r_i = m - 1 - 2^{m-2}. \tag{6.14}$$

Taking the moduli of both sides of (6.14) and using the triangle inequality gives

$$\sum_{i=3}^{m-1} |r_i| \geqq \left|\sum_{i=3}^{m-1} r_i\right| = 2^{m-2} - (m-1) > m - 2 \tag{6.15}$$

for $m \geqq 5$. Let $|r_{max}| = \max_i |r_i|$. Then (6.15) becomes

$$(m-3)|r_{max}| > m - 2,$$

so that $|r_{max}| > 1$ for $m \geqq 5$. This proves that the multistep method, and hence the corresponding spline solution, is divergent.

The above result is analogous to Theorem 2.6 in [8] concerning the application of high order splines to the numerical solution of the initial value problem (1.4). There it is pointed out that the unfortunate consequence of instability is due to the strictness of the continuity requirements in the spline function $S_m(x) \in C^{m-1}[a,b]$. However stable high order spline methods for numerically solving the initial value problem (1.4) are generated by relaxing the continuity restrictions through a more general definition of a spline function which allows

$$S(x) \in C^{k-1}[a,b],\ S(x) \notin C^{k}[a,b],\ k < m.$$

Analogous methods could possibly be described for the numerical solution of the boundary value problem (1.1).

Concerning the second question, we consider the general two-point boundary value problem

$$y'' = f(x,y,y'),\ y(a) = A,\ y(b) = B. \tag{6.16}$$

Following our development of the spline shooting technique, we would consider the related initial value problem

$$y'' = f(x,y,y'),\ y(a) = A,\ y'(a) = s, \tag{6.17}$$

where s is a parameter. Using the Taylor expansion method to construct a spline function approximation $S(x,s)$ to the solution $y(x,s)$ of (6.17) again would result in terms such as $y''(a,s) = f(a,A,s)$; that is, the parameter s enters in a nonlinear fashion. As discussed above, one could employ the usual shooting technique here also.

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VIII. ACKNOWLEDGEMENT

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