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ON THE CONVERGENCE OF SOME CUBIC SPLINE INTERPOLATION SCHEMES*

R. K. BEATSON†

Abstract. Cubic spline interpolation schemes which require no derivative information at the end points are of great practical importance and have been included in several general purpose software libraries. In this paper optimal order error estimates are developed for three popular schemes of this "derivative free" type. The approximation of $C^1[a,b]\backslash C^2[a,b]$ functions by any such "derivative free" method that reproduces cubics, necessarily displays some dependence on the local mesh ratio. However, for the spline interpolants studied here this dependence is restricted to the first and last subintervals.

Key words. spline, cubic spline, end conditions, endpoint phenomena, error estimates

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Introduction. Given data $\{(t_i, f(t_i))\}_{i=0}^n$ we will consider interpolatory

$$s(t_i)=f(t_i), \qquad 0 \leqq i \leqq n, \tag{1.1}$$

cubic splines s with knots $\mathbf{t}$. Two additional "end conditions" are needed to specify the spline completely. One choice of end conditions which has been the subject of intensive investigation is

$$s'(t_0)=f'(t_0) \quad \text{and} \quad s'(t_n)=f'(t_n), \tag{1.2}$$

corresponding to the complete spline (see Birkhoff and de Boor [1], Sharma and Meir [9], Hall [6] and de Boor [2]). This interpolant has many beautiful properties. However, derivatives of f are often unavailable so that end conditions not depending on derivative information are of great practical importance. A popular choice is the "not-a-knot" end condition,

$$s_-^{(3)}(t_1)=s_+^{(3)}(t_1) \quad \text{and} \quad s_-^{(3)}(t_{n-1})=s_+^{(3)}(t_{n-1}), \tag{1.3}$$

of de Boor [2]. This method is implemented in the widely used IMSL and NAG software libraries. Another practical choice is to force some derivative of s at t_0 and t_n to agree with that of a local cubic interpolant. For example, requiring

$$s'(t_0)=c_1'(t_0) \quad \text{and} \quad s'(t_n)=c_2'(t_n) \tag{1.4}$$

or

$$s''(t_0)=c_1''(t_0) \quad \text{and} \quad s''(t_n)=c_2''(t_n) \tag{1.5}$$

where c_1, c_2 are cubic polynomials such that

$$c_1(t_i)=f(t_i) \quad \text{and} \quad c_2(t_{n-i})=f(t_{n-i}), \qquad 0 \leqq i \leqq 3. \tag{1.6}$$

Swartz and Varga [10] show optimal order error estimates for the schemes (1.4) and (1.5) in the case of a quasi-uniform mesh and $f \in C^j[a,b]$, $0 \leqq j \leqq 3$. See also Forsythe, Malcolm and Moler [5, pp. 70–79].

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† Department of Mathematics, University of Connecticut, Storrs, Connecticut 06268. Present address, Mathematics Department, University of Canterbury, Christchurch 1, New Zealand.

For an application to monotone interpolation the author needed optimal order error estimates for such "derivative free" schemes in the case of an arbitrary mesh, and was surprised to learn at a July 1984 conference that these were not yet known. However, shortly thereafter, de Boor [3] showed the optimal error estimates for his "not-a-knot" scheme (1.3) when $f \in C^j[a, b]$, $2 \leqq j \leqq 3$. We will give a different proof of de Boor's result, and a proof of the analogous estimates for schemes (1.4), (1.5) below. We will also give optimal order error estimates for these schemes when f is merely C^1. These latter estimates display a dependence on the local mesh ratio in the first and last subintervals.

We will need the following notation. Let a knot set $\mathbf{t}$: $a = t_0 < t_1 < \cdots < t_n = b$ be given. A C^1 piecewise cubic on $\mathbf{t}$ is a $C^1[a, b]$ function which on each subinterval, (t_i, t_{i+1}), reduces to a cubic polynomial. A cubic spline, s, on $\mathbf{t}$ is a $C^2[a, b]$ function which on each subinterval, (t_i, t_{i+1}), reduces to a cubic polynomial. $g(\mathbf{t})$ denotes the vector $[g(t_0), \cdots, g(t_n)]^T$. $h_i = t_{i+1} - t_i$ is the length of the ith subinterval. $\delta = \max_{0 \leqq i \leqq n-1} h_i$ is the mesh length. $\theta_i = h_{i-1}/(h_{i-1} + h_i)$ expresses the relative lengths of adjacent subintervals. $\bar{\theta}_i = 1 - \theta_i$ for all i. $\|\cdot\|_{[c,d]}$ denotes the uniform norm for functions on the interval $[c, d]$. $\|\cdot\|$ without any subscripting interval denotes the uniform norm on $[a, b] = [t_0, t_n]$. $\omega(g, \varepsilon)$ denotes the usual uniform norm modulus of continuity of g on $[a, b]$. $|||\cdot|||$ denotes both the l_∞ norm for vectors and the corresponding operator norm for matrices. $g[t_i, t_{i+1}, \cdots, t_{i+k}]$ denotes the kth order divided difference of the function g over nodes $t_i, \cdots, t_{i+k}$. Throughout what follows, $C_1, C_2, C_3, \cdots$ denote positive constants which do not depend on the mesh $\mathbf{t}$ or the function f.

The various optimal order error estimates shown in §§ 2 and 3 below can be summarized by

THEOREM 1. *Given knots* $\mathbf{t}$ *with* $a = t_0 < t_1 < \cdots < t_n = b$, $n \geqq 5$, *and a function* f *defined on* $[a, b]$ *let* s *be the cubic spline interpolant corresponding to any one of the "derivative free" end conditions* (1.3), (1.4) *or* (1.5). *Then, if* $f \in C^1[a, b]$

$$\text{(1.7)} \quad \|(f-s)^{(k)}\|_{[t_i, t_{i+1}]} \leqq \begin{cases} C_1(1/\bar{\theta}_1) h_0^{1-k} \omega(f', \delta), & i = 0, \\ C_1 h_i^{1-k} \omega(f', \delta), & 1 \leqq i \leqq n-2, \quad k = 0, 1, \\ C_1(1/\theta_{n-1}) h_{n-1}^{1-k} \omega(f', \delta), & i = n-1. \end{cases}$$

The local mesh ratio dependent factors, $(1/\bar{\theta}_1)$ and $(1/\theta_{n-1})$, in (1.7) are essential. If $f \in C^j[a, b]$ for $j = 2$ or 3 then

$$\text{(1.8)} \quad \|(f-s)^{(k)}\|_{[t_i, t_{i+1}]} \leqq C_2 h_i^{2-k} \delta^{j-2} \omega(f^{(j)}, \delta), \qquad 0 \leqq i \leqq n-1, \quad k = 0, 1, 2.$$

It is shown below that any approximation scheme based on a finite sample of function values and reproducing cubic polynomials must display a mesh ratio dependent phenomenon in approximating functions that are merely C^1. What is remarkable is that this phenomenon can sometimes be confined to the first and last subintervals $[t_0, t_1]$ and $[t_{n-1}, t_n]$, as in (1.7).

2. Error bounds for cubic spline interpolation of functions in $C^2[a, b] \cup C^3[a, b]$. In this section we show the error estimates for the "derivative free" spline interpolation schemes (1.3), (1.4) and (1.5) and functions in $C^j[a, b]$, $j = 2$ or 3. Explicitly, we show for all 3 schemes

$$\text{(2.1)} \quad \|f^{(k)} - s^{(k)}\|_{[t_i, t_{i+1}]} \leqq C_3 h_i^{2-k} \delta^{j-2} \omega(f^{(j)}, \delta), \qquad 0 \leqq i \leqq n-1, \quad 0 \leqq k \leqq 2, \quad j = 2, 3.$$

Here, $n \geqq 3$ in the case of (1.4), (1.5), and $n \geqq 5$ in the case of (1.3). (2.1) implies the more usual but slightly weaker estimate $\|f^{(k)} - s^{(k)}\| = O(\delta^{j-k} \omega(f^{(j)}, \delta))$, $k = 0, 1, 2$, $j = 2, 3$.

In this section it is convenient to use the representation

$$p(x)=a_1\bar{w}+a_2w+a_3h^2(\bar{w}^3-\bar{w})/6+a_4h^2(w^3-w)/6 \tag{2.2}$$

for cubics on an interval $[t_i, t_{i+1}]$ where $w=(x-t_i)/h$, $\bar{w}=1-w$, and $h=h_i=(t_{i+1}-t_i)$. Actually, the coefficients are $a_1=p(t_i)$, $a_2=p(t_{i+1})$, $a_3=p''(t_i)$ and $a_4=p''(t_{i+1})$. Now, given $f(\mathbf{t})$ and any $(n+1)$ vector $\boldsymbol{\sigma}$, define a continuous piecewise cubic interpolant s to f as follows. On each subinterval $[t_i, t_{i+1}]$ let $s(x)=p(x)$ where $p(x)$ is given by (2.2) with $a_1=f(t_i)$, $a_2=f(t_{i+1})$, $a_3=\sigma_i$ and $a_4=\sigma_{i+1}$. Then s is a cubic spline (C^2) if and only if $s'_-(t_i)=s'_+(t_i)$, $1\leqq i\leqq n-1$, that is, if and only if

$$\theta_i\sigma_{i-1}+2\sigma_i+\bar{\theta}_i\sigma_{i+1}=6f[t_{i-1}, t_i, t_{i+1}], \qquad 1\leqq i\leqq n-1, \tag{2.3}$$

and then $\boldsymbol{\sigma}=s''(\mathbf{t})$. With this parametrization of s the end conditions (1.3), (1.4) and (1.5) are equivalent to

$$\begin{aligned}&-\bar{\theta}_1\sigma_0+\sigma_1-\theta_1\sigma_2=0,\\ &-\bar{\theta}_{n-1}\sigma_{n-2}+\sigma_{n-1}-\theta_{n-1}\sigma_n=0;\end{aligned} \tag{2.4}$$

$$\begin{aligned}&2\sigma_0+\sigma_1=6\{f[t_0, t_1, t_2]-(h_0+h_1)f[t_0, t_1, t_2, t_3]\},\\ &\sigma_{n-1}+2\sigma_n=6\{f[t_{n-2}, t_{n-1}, t_n]+(h_{n-2}+h_{n-1})f[t_{n-3}, t_{n-2}, t_{n-1}, t_n]\};\end{aligned} \tag{2.5}$$

and

$$\begin{aligned}&2\sigma_0=4f[t_0, t_1, t_2]-4f[t_0, t_1, t_2, t_3](2h_0+h_1),\\ &2\sigma_n=4f[t_{n-2}, t_{n-1}, t_n]+4f[t_{n-3}, t_{n-2}, t_{n-1}, t_n](2h_{n-1}+h_{n-2})\end{aligned} \tag{2.6}$$

respectively. It is now clear that fitting the spline subject to end conditions (1.3), (1.4) or (1.5) is equivalent to solving a linear system consisting of (2.3) combined with one of (2.4), (2.5) or (2.6) for $s''(\mathbf{t})$. We will need the following lemma.

LEMMA 2.1 (Sharma and Meir). *Consider cubic spline interpolation schemes of the following type. Given knots* $\mathbf{t}$: $a=t_0<t_1<\cdots<t_n=b$ *and a function* $f\in C^2[a, b]$, *let* s *be the cubic spline with these knots satisfying*

$$s(\mathbf{t})=f(\mathbf{t}) \quad \textit{and} \quad As^{(2)}(\mathbf{t})=g(f, \mathbf{t})$$

where A *is a nonsingular matrix and* g *is a function with range contained in* $\mathbb{R}^{n+1}$. *Then*

$$|||Af^{(2)}(\mathbf{t})-g(f, \mathbf{t})|||\leqq K\delta^{j-2}\omega(f^{(j)}, \delta), \qquad j=2, 3$$

implies

$$\|f^{(k)}-s^{(k)}\|_{[t_i,t_{i+1}]}\leqq(1+K|||A^{-1}|||)h_i^{2-k}\delta^{j-2}\omega(f^{(j)}, \delta), \qquad 0\leqq i\leqq n-1, 0\leqq k\leqq 2, j=2, 3.$$

Proof. Clearly, $|||f^{(2)}(\mathbf{t})-s^{(2)}(\mathbf{t})|||\leqq K|||A^{-1}|||\delta^{j-2}\omega(f^{(j)}, \delta)$. Since s is piecewise cubic, $s^{(2)}$ is piecewise linear. Let $\hat{s}^{(2)}$ be the piecewise linear interpolant to $f^{(2)}$ with knots $\mathbf{t}$. Then

$$\|f^{(2)}-s^{(2)}\|\leqq\|f^{(2)}-\hat{s}^{(2)}\|+\|\hat{s}^{(2)}-s^{(2)}\|\leqq\|f^{(2)}-\hat{s}^{(2)}\|+|||f^{(2)}(\mathbf{t})-s^{(2)}(\mathbf{t})|||.$$

This, together with the standard estimates for the error in piecewise linear interpolation, gives the result for $k=2$. The results for $k=0$ or 1 follow since both $e=f-s$ and e' have zeros in every subinterval $[t_i, t_{i+1}]$. □

2.1. Difference approximation end conditions. Consider cubic spline interpolation with end conditions (1.4) or (1.5), $n\geqq 3$. As discussed above this leads to a linear system $A\boldsymbol{\sigma}=\mathbf{b}$ for $\boldsymbol{\sigma}=s''(\mathbf{t})$. In either case we can show (2.1). We give the proof for end conditions (1.5). An analogous argument shows the estimates for end conditions

(1.4). The system (2.3) and (2.6) for $\boldsymbol{\sigma}$, $A\boldsymbol{\sigma}=\mathbf{b}$, is such that $A=2(I-B)$ where $|||B|||=\frac{1}{2}$. Hence $A^{-1}=\frac{1}{2}(I+B+B^2+\cdots)$ and $|||A^{-1}|||\leqq 1$. Also $|||Af^{(2)}(\mathbf{t})-\mathbf{b}|||$ is easily estimated by Taylor expansion to be $O(\delta^{j-2}\omega(f^{(j)},\delta))$, $j=2,3$ with an order constant not depending on the mesh. An application of Lemma 2.1 above gives the optimal order error estimate (2.1).

2.2. The not-a-knot end condition. Consider cubic spline interpolation with the end condition (1.3), $n\geqq 5$. As already mentioned the error estimate (2.1) for this scheme is due to de Boor [3] but we give a different proof below.

The linear system ((2.3), (2.4)), $A\boldsymbol{\sigma}=\mathbf{b}$, to be solved for $\boldsymbol{\sigma}=s''(\mathbf{t})$ is

$$\begin{aligned} &-\bar{\theta}_1\sigma_0+\sigma_1-\theta_1\sigma_2=0,\\ (2.7)\qquad &\theta_i\sigma_{i-1}+2\sigma_i+\bar{\theta}_i\sigma_{i+1}=6f[t_{i-1},t_i,t_{i+1}],\qquad 1\leqq i\leqq n-1.\\ &-\bar{\theta}_{n-1}\sigma_{n-2}+\sigma_{n-1}-\theta_{n-1}\sigma_n=0.\end{aligned}$$

The norm of A^{-1}, $|||A^{-1}|||$ is shown to be bounded independently of $\mathbf{t}$ in Lemma 2.2 below. Again, $|||Af^{(2)}(\mathbf{t})-\mathbf{b}|||$ is easily estimated by Taylor series expansion to be $O(\delta^{j-2}\omega(f^{(j)},\delta))$, $j=2,3$, with an order constant independent of the mesh $\mathbf{t}$. Estimate (2.1) follows from Lemma 2.1.

LEMMA 2.2. *There exists an absolute constant C_4 with the following property. Let $n\geqq 5$ be any integer and $0<\theta_i<1$, $1\leqq i\leqq n-1$ be any $n-1$ reals. Let $\bar{\theta}_i=1-\theta_i$ for all i. Then the matrix*

$$(2.8)\qquad A=\begin{bmatrix} -\bar{\theta}_1 & 1 & -\theta_1 & 0 & & & & \\ \theta_1 & 2 & \bar{\theta}_1 & 0 & & & & \\ 0 & \theta_2 & 2 & \bar{\theta}_2 & & & & \\ & & & & \ddots & & & \\ & & & & \theta_{n-2} & 2 & \bar{\theta}_{n-2} & 0 \\ & & & & 0 & \theta_{n-1} & 2 & \bar{\theta}_{n-1} \\ & & & & 0 & -\bar{\theta}_{n-1} & 1 & -\theta_{n-1} \end{bmatrix}$$

is nonsingular and $|||A^{-1}|||\leqq C_4$.

Proof. Consider the augmented matrix $[A:\mathbf{b}]$ corresponding to the system $A\mathbf{x}=\mathbf{b}$. If $0<\theta_1\leqq\frac{1}{2}$ then elementary row operations on the first three rows reduce them to the form

$$\begin{bmatrix} -\bar{\theta}_1 & 1 & -\theta_1 & 0 & 0 & \cdots & 0 & \hat{b}_0 \\ 0 & 2 & \xi & 0 & 0 & \cdots & 0 & \hat{b}_1 \\ 0 & 0 & 2 & \eta & 0 & \cdots & 0 & \hat{b}_2 \end{bmatrix}$$

where $|||\hat{\mathbf{b}}|||\leqq C_5|||\mathbf{b}|||$ and $0\leqq\xi,\ \eta\leqq 1$. Similarly, if $1/2<\theta_1<1$ then elementary row operations on the first three rows reduce them to

$$\begin{bmatrix} \theta_1 & 2 & \bar{\theta} & 0 & 0 & \cdots & \hat{b}_0 \\ 0 & 1 & -\xi & 0 & 0 & \cdots & \hat{b}_1 \\ 0 & 0 & 2 & \eta & 0 & \cdots & \hat{b}_2 \end{bmatrix}$$

where $\hat{\mathbf{b}}$, ξ, η satisfy the same inequalities as before.

Analogous operations can be carried out on the last three rows of $[A:\mathbf{b}]$. Now, introduce the notation $\mathbf{z}_*$ for the $n-3$ vector $[z_2, z_3,\cdots,z_{n-2}]^T$ derived from the $n+1$

vector $[z_0, z_1, \cdots, z_n]^T$. Then the original system $A\mathbf{x}=\mathbf{b}$ is equivalent to the partitioned system

$$(2.9) \qquad M\mathbf{x}_* = \hat{\mathbf{b}}_*, \quad \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = M_1 \begin{bmatrix} \hat{b}_0 \\ \hat{b}_1 \\ x_2 \end{bmatrix}, \quad \begin{bmatrix} x_{n-1} \\ x_n \end{bmatrix} = M_2 \begin{bmatrix} x_{n-2} \\ \hat{b}_{n-1} \\ \hat{b}_n \end{bmatrix},$$

where M is the $(n-3)\times(n-3)$ matrix

$$(2.10) \qquad \begin{bmatrix} 2 & \eta & & & & \\ \theta_3 & 2 & \bar{\theta}_3 & & & \\ & & \ddots & & & \\ & & & \theta_{n-3} & 2 & \bar{\theta}_{n-3} \\ & & & & \gamma & 2 \end{bmatrix},$$

and M_1, M_2 are 2×3 matrices of rank 2 with $|||M_i||| \leqq C_6$, $i=1,2$.

Now $M=2(I-B)$ where $|||B|||=\frac{1}{2}$. Hence $|||M^{-1}|||\leqq 1$. Thus, from (2.9) there is a unique solution $\mathbf{x}$ for any given $\mathbf{b}$, and $|||\mathbf{x}|||\leqq C_7|||\mathbf{b}|||$ for some constant C_7 not depending on the θ_i's. □

3. Error bounds for cubic spline interpolation of functions in $C^1[a, b]$. In this section we show optimal order error estimates for the derivative free interpolation methods (1.3), (1.4) and (1.5) and $f\in C^1[a, b]$. The estimates are necessarily dependent on the local mesh ratio in the first and last subintervals. Explicitly, we show

$$(3.1) \qquad \|(f-s)^{(k)}\|_{[t_i,t_{i+1}]} \leqq \begin{cases} C_8(1/\bar{\theta}_1)h_i^{1-k}\omega(f'\delta), & i=0, \\ C_8 h_i^{1-k}\omega(f', \delta), & 1\leqq i\leqq n-1, \quad k=0,1, \\ C_8(1/\theta_{n-1})h_i^{1-k}\omega(f', \delta), & i=n, \end{cases}$$

where $n\geqq 3$ in the case of (1.4), (1.5) and $n\geqq 4$ in the case of (1.3). The mesh dependent factor in inequality (3.1) cannot be removed. However, in the case of (1.4), (1.5), the factors $(1/\bar{\theta}_1)$ and $(1/\theta_{n-1})$ can be replaced by $(h_0/(h_1+h_2))$ and $(h_{n-1}/(h_{n-3}+h_{n-2}))$ respectively, yielding a stronger estimate.

Lemma 3.1 below shows that a mesh dependent term will appear in all estimates for $\|f'-g'\|_{[a,b]}$ in terms of $\omega(f', \delta)$, whenever the only information used in computing the approximation g is $\mathbf{t}$ and $f(\mathbf{t})$ and the approximation method reproduces cubics. There is no requirement that the operator g be a linear, or a spline, or an interpolatory operator for this result to hold. The complete spline, whose computation requires $f'(a)$ and $f'(b)$, does not exhibit this behavior and satisfies

$$\|(f-s)^{(k)}\|_{[t_i,t_{i+1}]} \leqq C_9 h_i^{1-k}\omega(f', \delta), \qquad 0\leqq i\leqq n-1, \quad k=0,1.$$

LEMMA 3.1. *There exists a positive constant C_{10} with the following property. Let $g(\mathbf{y}, \mathbf{t})$ be any continuous operator mapping $\mathbb{R}^{2n+2}$ into $C^1[a, b]$ and defined for all meshes $\mathbf{t}$ such that $a=t_0<t_1<\cdots<t_n=b$, $n\geqq N_0\geqq 3$, and arbitrary $\mathbf{y}\in\mathbb{R}^{n+1}$. Suppose*

$$(3.2) \qquad g(p(\mathbf{t}), \mathbf{t}) = p \quad \text{whenever } p\in\pi_3.$$

Then, given $0<\theta<\frac{1}{3}$, there exists for each $n\geqq N_0$ a mesh $\mathbf{t}$ with $\theta_i=\theta/(1+\theta)=\theta+O(\theta^2)$, $1\leqq i\leqq n-1$, and a nonconstant function $f\in C^1[t_0, t_n]$, such that

$$(3.3) \qquad \|g(f(\mathbf{t}), \mathbf{t})'\| \geqq C_{10}(1/\theta)\|f'\|.$$

An analogous result holds with $\bar{\theta}_i=\theta/(1+\theta)$ for all i.

Proof. Consider the mesh $\mathbf{t}$ with $t_i = \theta^{n-i}$, $0 \leqq i \leqq n$. The cubic $p(x) = x^2(1-x)$ satisfies

$$\max_{0\leqq i\leqq n-1} |p[t_i, t_{i+1}]| \leqq \max\left\{p'(\theta), \frac{p(\theta)}{1-\theta}\right\} \leqq 2\theta \tag{3.4}$$

and

$$|p[\tfrac{1}{2}, 1]| = \tfrac{1}{4}. \tag{3.5}$$

Replace p with its piecewise linear interpolant on the knots $\mathbf{t}$, q. Extend the definition of q to $[-1, 2]$ by linearity on the intervals $[-1, t_1]$ and $[t_{n-1}, 2]$. Note that q is absolutely continuous and $\|q'\|_\infty = \max_i |p[t_i, t_{i+1}]| \leqq 2\theta$. Smoothing q with the moving average yields $q_\varepsilon(x) = (1/2\varepsilon)\int_{-\varepsilon}^{\varepsilon} q(x+u)\,du$, $0 < \varepsilon < 1$. Note that $q_\varepsilon \in C^1[a, b]$,

$$\|q_\varepsilon'\| \leqq \|q'\|_\infty \leqq 2\theta, \tag{3.6}$$

and $\|q - q_\varepsilon\| \to 0$ as $\varepsilon \downarrow 0$. Since $g(q(\mathbf{t}), \mathbf{t}) = g(p(\mathbf{t}), \mathbf{t}) = p$, and the operator g is continuous, (3.5) implies we can choose an $\varepsilon > 0$ sufficiently small that

$$\|g(q_\varepsilon(\mathbf{t}), \mathbf{t}))'\| \geqq |g(q_\varepsilon(\mathbf{t}), \mathbf{t})[\tfrac{1}{2}, 1]| \geqq \tfrac{1}{8}. \tag{3.7}$$

Choosing $f = q_\varepsilon$, (3.6) and (3.7) give the lemma. □

In this section it is convenient to use the representation

$$p(x) = p(t_i)\bar{w}^2(2w+1) + p(t_{i+1})w^2(2\bar{w}+1) + p'(t_i)hw\bar{w}^2 - p'(t_{i+1})h\bar{w}w^2 \tag{3.8}$$

for cubics on the interval $[t_i, t_{i+1}]$ where $w = (x - t_i)/h$, $\bar{w} = 1 - w$ and $h = h_i = (t_{i+1} - t_i)$. Now given $f(\mathbf{t})$ and any $(n+1)$ vector $\boldsymbol{\lambda}$, define a continuously differentiable piecewise cubic interpolant s to f as follows. On each subinterval $[t_i, t_{i+1}]$ let $s(x) = p(x)$ where $p(x)$ is the cubic with $p(t_i) = f(t_i)$, $p(t_{i+1}) = f(t_{i+1})$, $p'(t_i) = \lambda_i$ and $p'(t_{i+1}) = \lambda_{i+1}$. Then s is cubic spline if and only if $s''_-(t_i) = s''_+(t_i)$, $1 \leqq i \leqq n-1$. That is, if and only if

$$\bar{\theta}_i\lambda_{i-1} + 2\lambda_i + \theta_i\lambda_{i+1} = 3(\bar{\theta}_i f[t_{i-1}, t_i] + \theta_i f[t_i, t_{i+1}]), \qquad 1 \leqq i \leqq n-1, \tag{3.9}$$

where $\boldsymbol{\lambda} = s'(\mathbf{t})$. With this parametrization of s the end conditions (1.3), (1.4) and (1.5) are equivalent to

$$\begin{aligned} &\bar{\theta}_1\lambda_0 + \lambda_1 = \bar{\theta}_1(2+\theta_1)f[t_0, t_1] + \theta_1^2 f[t_1, t_2], \\ &\lambda_{n-1} + \theta_{n-1}\lambda_n = \bar{\theta}_{n-1}^2 f[t_{n-2}, t_{n-1}] + \theta_{n-1}(2+\bar{\theta}_{n-1})f[t_{n-1}, t_n]; \end{aligned} \tag{3.10}$$

$$\begin{aligned} 2\lambda_0 &= 2f[t_0, t_1] - 2h_0 f[t_0, t_1, t_2] + 2h_0(h_0+h_1)f[t_0, t_1, t_2, t_3], \\ 2\lambda_n &= 2f[t_{n-1}, t_n] + 2h_{n-1}f[t_{n-2}, t_{n-1}, t_n] \\ &\qquad + 2h_{n-1}(h_{n-2}+h_{n-1})f[t_{n-3}, t_{n-2}, t_{n-1}, t_n]; \end{aligned} \tag{3.11}$$

and

$$\begin{aligned} 2\lambda_0 + \lambda_1 &= 3f[t_0, t_1] - h_0 f[t_0, t_1, t_2] + h_0(2h_0+h_1)f[t_0, t_1, t_2, t_3], \\ \lambda_{n-1} + 2\lambda_n &= 3f[t_{n-1}, t_n] + h_{n-1}f[t_{n-2}, t_{n-1}, t_n] \\ &\qquad + h_{n-1}(2h_{n-1}+h_{n-2})f[t_{n-3}, t_{n-2}, t_{n-1}, t_n] \end{aligned} \tag{3.12}$$

respectively. Fitting the spline subject to end conditions (1.3), (1.4) or (1.5) can now be formulated as solving a linear system consisting of (3.9) combined with (3.10), (3.11) or (3.12) respectively. We will need the following lemma.

LEMMA 3.2. *Let $p(x)\in\pi_3$ interpolate $f\in C^1[c,d]$ at c and d and satisfy*

$$\max\{|f'(c)-p'(c)|,|f'(d)-p'(d)|\}\leqq\varepsilon.$$

Then

$$\|f'-p'\|_{[c,d]}\leqq\frac{7}{2}\omega\left(f',\frac{d-c}{2}\right)+\varepsilon \qquad \textit{iff}\in C^1[c,d], \tag{3.13i}$$

$$\|f'-p'\|_{[c,d]}\leqq\frac{7}{4}(d-c)\omega\left(f'',\frac{d-c}{2}\right)+\varepsilon \qquad \textit{iff}\in C^2[c,d], \tag{3.13ii}$$

$$\|f'-p'\|_{[c,d]}\leqq\frac{7}{8}(d-c)^2\omega\left(f^{(3)},\frac{d-c}{2}\right)+\varepsilon \qquad \textit{iff}\in C^3[c,d], \tag{3.13iii}$$

and

$$\|f-p\|_{[c,d]}\leqq\left(\frac{d-c}{2}\right)\|f'-p'\|_{[c,d]}. \tag{3.14}$$

Proof. It is sufficient to prove the result when $[c,d]=[0,1]$. Let $L(f)$ be the Hermite cubic interpolant to f at c and d,

$$\begin{aligned}L(f)&=f(c)\bar{w}^2(2w+1)+f(d)w^2(2\bar{w}+1)+f'(c)hw\bar{w}^2-f'(d)h\bar{w}w^2\\&=f(c)\phi_{00}(x)+f(d)\phi_{10}(x)+f'(c)\phi_{01}(x)+f'(d)\phi_{11}(x),\end{aligned}$$

where here $c=0$, $d=1$, $w=x$, $\bar{w}=1-x$ and $h=1$. If we define the derived projector $L'\colon f'\to\pi_2$ by $L'(f')=(Lf)'$ then a calculation shows

$$L'(f',\tfrac{1}{2})=\tfrac{3}{2}\int_0^1 f'(t)\,dt-\tfrac{1}{4}(f'(0)+f'(1)), \tag{3.15}$$

so $|L'(f',\frac{1}{2})|\leqq 2\|f'\|_{[0,1]}$. But it is well known (de Boor [2, p. 61] or Cheney [4, p. 65]) that for quadratics q $\|q\|_{[0,1]}\leqq\frac{5}{4}\max\{|q(0)|,|q(\frac{1}{2})|,|q(1)|\}$. Hence $\|L'\|\leqq\frac{5}{2}$. Now

$$\begin{aligned}\|f'-p'\|_{[0,1]}&\leqq\|f'-(Lf)'\|_{[0,1]}+\|(Lf)'-p'\|_{[0,1]}\\&\leqq(1+\|L'\|)\operatorname{dist}(f',\pi_2)+\varepsilon\|\,|\phi'_{01}(x)|+|\phi'_{11}(x)|\,\|_{[0,1]}\end{aligned}$$

and estimating $\operatorname{dist}(f',\pi_2)$ with Taylor's theorem in the form (Shapiro [8, p. 53])

$$\left|g(x+t)-\sum_{k=0}^{r}\frac{g^{(k)}(x)t^k}{k!}\right|\leqq\frac{|t|^r}{r!}\omega(g^{(r)},|t|)$$

we find (3.13). (3.14) follows since $(f-p)(0)=(f-p)(1)=0$. □

3.1. Difference approximation end conditions. In this section we show the error estimates (3.1) for cubic spline interpolation with end conditions (1.5). An analogous argument shows the estimates for end conditions (1.4).

The system determining $\boldsymbol{\lambda}=s'(\mathbf{t})$ ((3.9), (3.12)) is $A\boldsymbol{\lambda}=\mathbf{b}$ where

$$A=\begin{bmatrix}2&1&&&&&\\\bar{\theta}_1&2&\theta_1&&&&\\&\bar{\theta}_2&2&\theta_2&&&\\&&&\ddots&&&\\&&&&\bar{\theta}_{n-1}&2&\theta_{n-1}\\&&&&&1&2\end{bmatrix} \tag{3.16}$$

and

$$(3.17)\qquad b_i=\begin{cases}3f[t_0,t_1]-h_0f[t_0,t_1,t_2]+h_0(2h_0+h_1)f[t_0,t_1,t_2,t_3], & i=0,\\ 3(\bar\theta_if[t_{i-1},t_i]+\theta_if[t_i,t_{i+1}]), & 1\leqq i\leqq n-1,\\ 3f[t_{n-1},t_n]+h_{n-1}f[t_{n-2},t_{n-1},t_n] & \\ \qquad +h_{n-1}(2h_{n-1}+h_{n-2})f[t_{n-3},t_{n-2},t_{n-1},t_n], & i=n.\end{cases}$$

Let $e=f-s$. Then $Ae'(\mathbf{t})=Af'(\mathbf{t})-\mathbf{b}=\mathbf{r}$ and by a Taylor series expansion

$$(3.18)\qquad |r_i|\leqq\begin{cases}C_{11}\max\left\{1,\dfrac{h_0}{h_1+h_2}\right\}\omega(f',\delta)\leqq C_{11}(1/\bar\theta_1)\omega(f',\delta), & i=0,\\ C_{11}\omega(f',\delta), & 1\leqq i\leqq n-1,\\ C_{11}\max\left\{1,\dfrac{h_{n-1}}{h_{n-3}+h_{n-2}}\right\}\omega(f',\delta)\leqq C_{11}(1/\theta_{n-1})\omega(f',\delta), & i=n.\end{cases}$$

Introduce the notation $\mathbf{z}_{\#}$ for the $(n-1)$-vector $[z_1,z_2,\cdots,z_{n-1}]^T$ derived from the $n+1$ vector $[z_0,z_1,\cdots,z_n]^T$. The system $Ae'(\mathbf{t})=\mathbf{r}$ is equivalent to the partitioned system

$$(3.19)\qquad B\mathbf{e}'_{\#}=\hat{\mathbf{r}}_{\#},\quad 2e'_0+e'_1=r_0,\quad e'_{n-1}+2e'_n=r_n$$

where

$$B=\begin{bmatrix}2-0.5\bar\theta_1 & \theta_1 & & & & \\ \bar\theta_2 & 2 & \theta_2 & & & \\ & & \ddots & & & \\ & & & \bar\theta_{n-2} & 2 & \theta_{n-2}\\ & & & & \bar\theta_{n-1} & 2-0.5\theta_{n-1}\end{bmatrix}$$

and

$$\hat r_i=\begin{cases}r_1-0.5\bar\theta_1r_0, & i=1,\\ r_i, & 2\leqq i\leqq n-2,\\ r_{n-1}-0.5\theta_{n-1}r_n, & i=n-1.\end{cases}$$

Thus from (3.18), $|\hat r_i|\leqq C_{12}\omega(f',\delta)$, $1\leqq i\leqq n-1$. Standard diagonal dominance arguments show $|||B^{-1}|||$ is bounded independently of the mesh. Hence $|||\mathbf{e}'_{\#}|||\leqq C_{13}\omega(f',\delta)$. Combining this with (3.19) and (3.18)

$$(3.20)\qquad |e'_i|\leqq\begin{cases}C_{14}\max\left\{1,\dfrac{h_0}{h_1+h_2}\right\}\omega(f',\delta), & i=0,\\ C_{14}\omega(f',\delta), & 1\leqq i\leqq n-1,\\ C_{14}\max\left\{1,\dfrac{h_{n-1}}{h_{n-3}+h_{n-2}}\right\}\omega(f',\delta), & i=n.\end{cases}$$

The result follows on applying Lemma 3.2 on each subinterval $[t_i,t_{i+1}]$.

The following example shows that the estimate of the mesh dependent behavior given in (3.20), and thus in the improved form of (3.1), is essentially best possible. This example concerns the behavior of $s'(t_0)$. An analogous example can be given for $s'(t_n)$. Let $0<\varepsilon<1$ and $t_0=0<t_1=1<t_2<t_3=1+\varepsilon<t_4<\cdots<t_n$. Hence $h_0/(h_1+h_2)=1/\varepsilon$. Consider a function $f\in C^1[a,b]$ such that $f[t_1,t_2]=1$ and $f[t_i,t_{i+1}]=0$, $i\neq 1$. It is easy to show that there exists such an f with $\|f'\|<1+\varepsilon$. Now, if s is the spline (1.5) fitted to this data, then since $\omega(f',\delta)\leqq 2\|f'\|$, (3.1) shows $|s'(t_1)|=O(1)$. Hence by (3.12) $s'(t_0)=-1/\varepsilon+O(1)=-h_0/(h_1+h_2)+O(1)$ as $\varepsilon\downarrow 0$.

3.2. The not-a-knot end condition. In this section we show the error estimates (3.1) for the "not-a-knot" cubic spline interpolant.

The system determining $\boldsymbol{\lambda} = s'(\mathbf{t})$ ((3.9), (3.10)) is $A\boldsymbol{\lambda} = \mathbf{b}$ where

$$A = \begin{bmatrix} \bar\theta_1 & 1 & & & & & \\ \bar\theta_1 & 2 & \theta_1 & & & & \\ & \bar\theta_2 & 2 & \theta_2 & & & \\ & & & \ddots & & & \\ & & & & \bar\theta_{n-1} & 2 & \theta_{n-1} \\ & & & & & 1 & \theta_{n-1} \end{bmatrix} \tag{3.21}$$

and

$$b_i = \begin{cases} \bar\theta_1(2+\theta_1)f[t_0, t_1] + \theta_1^2 f[t_1, t_2], & i = 0, \\ 3(\bar\theta_i f[t_{i-1}, t_i] + \theta_i f[t_i, t_{i+1}]), & 1 \leqq i \leqq n-1, \\ \bar\theta_{n-1}^2 f[t_{n-2}, t_{n-1}] + \theta_{n-1}(2+\bar\theta_{n-1}) f[t_{n-1}, t_n], & i = n. \end{cases} \tag{3.22}$$

Let $e = f - s$. Then $Ae'(\mathbf{t}) = Af'(\mathbf{t}) - \mathbf{b} = \mathbf{r}$ and by Taylor series expansion

$$|r_i| \leqq C_{15}\omega(f', \delta), \qquad 0 \leqq i \leqq n. \tag{3.23}$$

The system $Ae'(\mathbf{t}) = \mathbf{r}$ is equivalent to the partitioned system

$$B\mathbf{e}'_{\#} = \hat{\mathbf{r}}_{\#}, \quad \bar\theta_1 e'_0 + e'_1 = r_0, \quad e'_{n-1} + \theta_{n-1} e'_n = r_n \tag{3.24}$$

where

$$B = \begin{bmatrix} 1 & \theta_1 & & & & & \\ \bar\theta_2 & 2 & \theta_2 & & & & \\ & \bar\theta_3 & 2 & \theta_3 & & & \\ & & & \ddots & & & \\ & & & & \bar\theta_{n-2} & 2 & \theta_{n-2} \\ & & & & & \bar\theta_{n-1} & 1 \end{bmatrix}$$

and

$$\hat r_i = \begin{cases} r_1 - r_0, & i = 1, \\ r_i, & 2 \leqq i \leqq n-2, \\ r_{n-1} - r_n, & i = n-1. \end{cases}$$

Kershaw [7] gives useful estimates for the inverses of certain tridiagonal matrices. In particular, these estimates show that $|||B^{-1}|||$ is bounded independently of $\theta_1, \theta_2, \cdots, \theta_n$. Hence from (3.23) $|||\mathbf{e}'_{\#}||| \leqq C_{16}\omega(f', \delta)$ and by (3.24)

$$|e'_i| \leqq \begin{cases} C_{17}(1/\bar\theta_1)\omega(f', \delta), & i = 0, \\ C_{17}\omega(f', \delta), & 1 \leqq i \leqq n-1, \\ C_{17}(1/\theta_{n-1})\omega(f', \delta), & i = n. \end{cases} \tag{3.25}$$

The result follows on applying Lemma 3.2 on each subinterval $[t_i, t_{i+1}]$.

The following example shows that the estimate of the mesh dependent behavior given in (3.25), and thus in (3.1) is essentially best possible. In the example we estimate $s'(t_0)$ but a similar example exists for $s'(t_n)$.

From Kershaw's estimates for the elements of B^{-1}, and the elementary fact that the jth column of A^{-1} is the solution $\mathbf{x}$ of $A\mathbf{x} = \mathbf{e}_j$, we find

$$a_{00}^{-1} = (1+c)/\bar\theta_1, \qquad a_{01}^{-1} = -c/\bar\theta_1, \qquad \theta_1/(2\bar\theta_1) < a_{02}^{-1} < \theta_1/\bar\theta_1,$$

where $c = b_{11}^{-1}$ and $1 < c < 2$.

Now take $\frac{1}{2} > \varepsilon > 0$ and $t_0 = 0 < t_1 = 1 < t_2 = 1 + \varepsilon < t_3 = 1 + \frac{4}{3}\varepsilon < t_4 < \cdots < t_n$. Hence $\theta_1 = 1/(1+\varepsilon)$, $\bar{\theta}_1 = \varepsilon + O(\varepsilon^2)$, $\bar{\theta}_2 = \frac{1}{4}$. Consider a function $f \in C^1[a, b]$ with $f[t_1, t_2] = 1$ and $f[t_i, t_{i+1}] = 0$, $i \neq 1$. As in the previous section such a function exists with $\|f'\| \leqq 1 + \varepsilon$. Now, using (3.22)

$$\begin{aligned} s'(t_0) &= a_{00}^{-1}\theta_1^2 + a_{01}^{-1} 3\theta_1 + a_{02}^{-1} 3\bar{\theta}_2 \\ &\leqq (\theta_1/\bar{\theta}_1)[(1+c) - 3c + \tfrac{3}{4}] < -1/(8\bar{\theta}_1), \end{aligned}$$

since $1 < c < 2$ and $\theta_1 > \frac{1}{2}$. Hence the factor $1/\bar{\theta}_1$ in (3.25) cannot be replaced by anything smaller in general.

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