PIECEWISE POLYNOMIAL INTERPOLATION, PARTICULARLY WITH CUBIC SPLINES

1. Setup. Everything we do with piecewise-polynomial approximation will be set in the following more-or-less standard framework. We are given $(n+1)$ nodes, usually numbered from left to right,

$$a = x_0 < x_1 < \cdots < x_n = b$$

which divide the interval $J = [x_0, x_n]$ into n cells, the i-th being $J_i = [x_i, x_{i+1}]$ of length $h_i = x_{i+1} - x_i > 0$. Implicitly we are given a function $f(x)$ defined on J. We seek n polynomials $\{p_i(x) : i = 0, \ldots, n-1\}$ which will define a function "near" $f(x)$ by defining the "nearby" function as equal to $p_i(x)$ on the cell $[x_i, x_{i+1}]$. Thus there is no "single analytic definition" for the approximating function—one has to know the cell in which x lies in order to evaluate the approximating function at x. All the polynomials $p_i(x)$ will have the same degree, however—indeed, in the most important case they will all be cubics—and the "nearness" will include the requirement that the piecewise polynomial function they define interpolate $f(x)$ on the nodes, so that

$$p_0(x_0) = f(x_0) = f_0,\ p_0(x_1) = p_1(x_1) = f(x_1) = f_1,\ \ldots,\ p_{n-1}(x_{n-1}) = f(x_{n-1}) = f_{n-1},$$
$$\text{and moreover,}\ \ p_{n-1}(x_n) = f(x_n) = f_n\ .$$

Thus each polynomial satisfies two interpolation conditions, and in addition to those there may be "end conditions" at $x_0 = a$ and $x_n = b$ and conditions that link the "pieces" at the nodes. When we need a name for the function defined on all of J by using the polynomial pieces, we call it $s(x)$; the piece defined on J_i will be called $p_i(x)$. When we need a single estimate for the lengths of the cells, we use $h = \max_i\{|h_i| : 0 \le i < n\}$.

We shall tacitly assume that the function $f(x)$ has as much differentiability as it needs to make our theorems make sense. In particular, functions to be interpolated by cubic splines will usually be assumed to be twice-continuously differentiable at least, and sometimes "twice" will be replaced by "four-" or "five-times." People who know what these things are will realize that in some situations it would suffice that the functions have distributional derivatives that belong to $L^2(J)$ (buzzword = *Sobolëv space*).

{Remark: The convention used above to number intervals J_i and increments h_i numbers the intervals by their left-hand endpoints. This convention conforms to Atkinson's book, but you should note that Stoer & Bulirsch [for example] number by r. h. endpoints. I feel that numbering by r. h. endpoints is better for coding purposes, but the reason for this feeling is probably that the early versions of `Fortran` were unwilling to admit zero as the value of an index. Possibly `C` programming would be easier with the intervals indexed from 0 to $n-1$. In all cases, though, I see no reason gratuitously to fight the textbook on this matter.}

2. Lower-degree and Uncoupled Examples. Here are some simple cases of piecewise polynomial approximation. If all the $p_i(x)$'s are linear, then just the requirement that $p_i(x)$ interpolate the values of $f(x)$ at the endpoints of J_i uniquely determines the polynomial $p_i(x)$: there is only one linear interpolant between the two values at x_i and x_{i+1}. The function $s(x)$ is thus uniquely determined. An estimate of its deviation from $f(x)$ can be made on an interval-by-interval basis: in J_i we can write

$$f(x) = p_i(x) + \frac{f''(\xi_x)}{2!}(x - x_i)(x - x_{i+1})\ .$$

The maximum value of $|(x - x_i)(x - x_{i+1})|$ is $\dfrac{h_i^2}{4}$, attained at the midpoint of J_i. We thus have a global, uniform error estimate

$$|f(x) - s(x)| \le \frac{M_2}{2} \cdot \frac{h^2}{4}$$

where $M_2 = \max\{|f''(x)| : x \in J\}$. The object we have constructed is called the **piecewise-linear interpolant** of $f(x)$, for obvious reasons.

The next case would be to take all the $p_i(x)$'s quadratic, and a natural first hope would be that we might be able to match up the first derivative of $s(x)$ with that of $f(x)$ at the nodes. That hope does not long survive the following count. If all the $p_i(x)$'s are quadratic, then there are $3n$ coefficients required in order completely to determine $s(x)$. The requirement that $p_i(x)$ take the same values as $f(x)$ at each node imposes 2 conditions on each $p_i(x)$; there are n intervals, so that requires the coefficients to satisfy $2n$ linear equations. If we simply want to have $s'(x)$ continuous at each of the interior nodes $x_1, \ldots, x_{n-1}$, we impose an additional $(n-1)$ equations

$$p_i'(x_{i+1}) = p_{i+1}'(x_{i+1}), \quad i = 0, \ldots, n-2$$

that the coefficients must satisfy: we have imposed $2n + (n-1) = 3n - 1$ linear conditions on the coefficients, and we would expect that "there is only one degree of freedom remaining." Certainly an attempt to make $s'(x_i) = f'(x_i)$ at each node would add $(n+1)$ equations, bringing the count to $4n$, and it does not seem reasonable to expect such a heavily overdetermined a set of equations in $3n$ unknowns to have a solution at all.

In fact, it is easy to see what the remaining degree of freedom is. Given an interval $[\alpha, \beta]$ and some number γ, there is a unique quadratic polynomial $q(x)$ that interpolates $f(x)$ at the endpoints and has $q'(\alpha) = \gamma$; in Newton form that polynomial is

$$q(x) = f(\alpha) + \gamma \cdot (x - \alpha) + \frac{f[\alpha, \beta] - \gamma}{\beta - \alpha} \cdot (x - \alpha)^2$$

as the reader may see by constructing a divided-difference table. One can now compute

$$q'(\beta) = 2 \cdot f[\alpha, \beta] - \gamma$$

directly. So if in piecewise-quadratic interpolation we specify a value for $p_0'(x_0) = s'(x_0)$, then $p_0'(x_1)$ is determined, and if $s'(x)$ is to be continuous at x_1 then $p_1'(x_1)$ is determined ... and so on down the line; specifying the derivative at x_0 has taken away the one degree of freedom left in the choice of $s(x)$. {Take $[\alpha, \beta]$ successively to equal $[x_0, x_1]$, $[x_1, x_2]$, ...} The coefficients of the $p_i(x)$'s are "coupled" at the nodes by the requirement that $s'(x)$ be continuous, but they're not coupled in a very complicated way: one can see the single choice that one makes in order to determine the entire cubic spline uniquely move from left to right along the interval as one computes the successive $p_i(x)$'s in Newton form (which incidentally happens to be the same as Taylor form in this case).

Although a piecewise quadratic can be made $\mathcal{C}^1$ and it is more complicated than a piecewise linear function, it is not clear that it approximates $f(x)$ any better; in fact, by thinking of an extremely inept choice of $s'(x_0)$ you can easily convince yourself that it may be a *worse* approximation! {Suppose $f(x)$ is a constant function: if $s'(x_0) \neq 0$ then the piecewise-quadratic will oscillate around the constant, while the piecewise-linear would equal the constant. Of course that was a loaded example—but suppose $f(x)$ wiggles a little in J_0 but is constant in $[x_1, x_n]$. Then even matching $s'(x_0)$ and $f'(x_0)$ may not help.} If we are to have $s'(x)$ behave nicely with respect to $f'(x)$—in addition to being continuous—it appears that we shall need more freedom than the one degree that piecewise-quadratic functions would furnish. So on we go to piecewise-cubic interpolation.

If all the $p_i(x)$ are to be cubics, then it will require $4n$ coefficients to determine all the polynomials. The requirement that the piecewise function they define be an interpolant of $f(x)$ imposes $2(n-1) + 2 = 2n$ conditions, all of which can be expressed linearly in the coefficients and which look as if they should be linearly independent. In **piecewise-cubic Hermite interpolation** we require that the first derivative of the i-th interpolating polynomial interpolate the derivative of $f(x)$ at the nodes. This imposes $2n$ additional conditions and determines the $p_i(x)$'s uniquely. Indeed, finding the $p_i(x)$'s then becomes a purely "local" problem: one finds the cubic Hermite interpolant of $f(x)$ on $[x_i, x_{i+1}]$ and that is $p_i(x)$; no interaction between cells takes place.

The whole situation is exactly analogous to piecewise-linear interpolation; all that happens is that the first derivative is interpolated along with the function. To see what happens on a single interval, look at Atkinson's treatment of Hermite interpolation on a single interval $[a, b]$, which is the example on pp. 162–163.

Note that here we do have a good error estimate: applying Atkinson's formula (3.6.15) piece-by-piece gives us

$$|f(x) - s(x)| \le \frac{M_4}{384} \cdot h^4$$

where $M_4 = \max\{|f^{(4)}(x)| : x_0 \le x \le x_n\}$. The error $\to 0$ as $h \to 0$ twice as fast as the error for piecewise-linear interpolation did, and it is nice to have the factor $\dfrac{1}{384} \approx 10^{-2.6}$ in there to help make the error smaller too. In general, however, one will have $p''_{i-1}(x_i) \ne p''_i(x_i)$, $i = 1, \ldots, n-1$; the first derivative of the interpolant is continuous, but there will usually be jumps in its second derivative (which is not well-defined at the nodes).

The definition of **cubic splines** is made (at least partly) in order to avoid those discontinuities: the idea is that we will force the piecewise cubic to be an interpolant of $f(x)$ but will force the equalities

$$p''_{i-1}(x_i) = p''_i(x_i) \qquad i = 1, \ldots, n-1$$

so as to get a continuous second derivative. That already gives $2n + (n-1) = 3n-1$ conditions on the coefficients, so there is not enough freedom remaining to force the first derivatives to agree with $f'(x)$ at the nodes. What one can do is to force the first derivatives of the cubic pieces to agree with each other at the nodes:

$$p'_{i-1}(x_i) = p'_i(x_i) \qquad i = 1, \ldots, n-1 \; .$$

This gives $n-1$ additional conditions, bringing the count up to $(3n-1) + (n-1) = 4n-2$. While the common values $\{b_i : i = 1, \ldots, n-1\}$ of the first derivatives will probably not satisfy $b_i = f'(x_i)$, we may hope that the difference will be fairly small if $f(x)$ is sufficiently smooth and if the $\{h_i\}_{i=0}^{n-1}$ are sufficiently small. One expects that 2 additional conditions are needed if all the pieces of the piecewise cubic interpolant are to be determined uniquely. While there is no canonical choice of these conditions, three popular choices are

(1) The **Complete Cubic Spline Interpolant**, produced by choosing

$$p'_0(x_0) = f'(x_0) \quad \text{and} \quad p'_{n-1}(x_n) = f'(x_n) \; ;$$

"the first derivative is correct at the endpoints."

(2) The **Natural Cubic Spline Interpolant**, produced by choosing the $\{b_i\}$ so that

$$p''_0(x_0) = 0 \quad \text{and} \quad p''_{n-1}(x_n) = 0 \; ;$$

"no curvature is present at the endpoints." It can be argued that this is not at all natural, since $f''(x)$ need not be zero at the endpoints, and indeed the error estimates for this interpolant are not as small as those for the complete spline. (While it is not obvious that this condition can be produced by a suitable choice of the $\{b_i\}$, we shall see later that it can be.)

(3) The **Periodic Cubic Spline Interpolant**, produced by choosing the $\{b_i\}$ so that

$$p'_0(x_0) = p'_n(x_n) \quad \text{and} \quad p''_0(x_0) = p''_n(x_n) \; ;$$

it is most natural to use these conditions with a function for which $f(x_0) = f(x_n)$, so that the function $f(x)$ "wants to have a periodic extension" to the real line with period cells that are the translates of J. {Of course a function can have periodic derivatives without itself being periodic; the interested reader may want to contemplate the situation further.}

Atkinson (pp. 166–176) deals with the natural cubic spline interpolant, (2) above. These notes will deal with the complete cubic spline interpolant, (1) above; error estimates are fairly straightforward to make and make best possible, and the natural spline can then be treated as a perturbed version of the complete spline. Periodic splines will largely be left to the reader.

3. Notational Differences Between these notes and Atkinson pp. 166–176.

Atkinson denotes the function value at x_i by y_i; these notes use f_i.

Atkinson writes, but never uses, the form

$$s(x) = a_i + b_i x + c_i x^2 + d_i x^3 \quad \text{for } x_{i-1} \leq x \leq x_i \;; .$$

We shall implicitly use, but rarely write, the form

$$p_i(x) = f_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$$

for the i-th polynomial written in Taylor form with base point equal to x_i, the left endpoint of the i-th cell. Note that the equations

Atkinson	|	These notes
$y_i = s(x_i)$	$=$	f_i
$s'(x_i)$	$=$	b_i
$M_i = s''(x_i)$	$=$	$2! \cdot c_i$
$s^{(3)}(x_i)$	$=$	$3! \cdot d_i$

connect the values and derivatives of the spline with the coefficients of $p_i(x)$ when the latter is written in Taylor form.

4. Cubic Spline Interpolants as the Solution of a Variational Problem. It is a remarkable fact that the existence and uniqueness of cubic spline interpolants, as well as some of their approximation properties, can be established in a nonconstructive way. {Why do something nonconstructive in a course in numerical analysis? Because it illustrates the idea of finding solutions by solving variational problems, which is an important idea in applied mathematics generally, and one which recurs in the finite-element method for numerical solution of boundary value problems of differential equations.} The basic lemma is sometimes called *Holladay's identity.*}

Lemma: In the general setup of these notes, let $f(x)$ be twice continuously differentiable. Suppose $s(x)$ is a cubic spline interpolant of $f(x)$ that satisfies either the natural-interpolant endpoint conditions

$$s''(x_0) = 0 \quad \text{and} \quad s''(x_n) = 0 \;,$$

the complete-interpolant endpoint conditions

$$s'(x_0) = f'(x_0) \quad \text{and} \quad s'(x_n) = f'(x_n) \;,$$

or the periodic endpoint conditions (assuming also that $f(x_0) = f(x_n)$)

$$s'(x_0) = s'(x_n) \quad \text{and} \quad s''(x_0) = s''(x_n) \;.$$

If $g(x)$ is any $\mathcal{C}^2$-function that interpolates $f(x)$ at the nodes $\{x_i\}$ (including $f(x)$ itself), then

$$\int_{x_0}^{x_n} |g''(x)|^2 \, dx = \int_{x_0}^{x_n} |s''(x)|^2 \, dx + \int_{x_0}^{x_n} |s'' - g''|^2 \, dx$$

holds when $s(x)$ satisfies the natural-interpolant endpoint conditions. The same is true for the complete spline interpolant $s(x)$ if $g(x)$ also satisfies the "complete endpoint conditions" $g'(x_0) = f'(x_0)$ and $g'(x_n) = f'(x_n)$, and is true for the periodic spline interpolant if $g'(x_0) = g'(x_n)$.

Non-Digression Before the Proof. Having spent some time in Hilbert space, we should recognize that anything involving the integral of the square of a function, like $\int_{x_0}^{x_n} |g''(x)|^2\,dx$, really involves an "inner product," in this case having the form

$$\langle f, g\rangle = \int_{x_0}^{x_n} f''(x)\overline{g''(x)}\,dx\ .$$

This is not (strictly speaking) an inner product, but rather a "quadratic form" defined on pairs of functions f, g—which for our present purposes(1) we can take as belonging to $\mathcal{C}^2([a,b])$. Unlike the familiar inner product that does not involve derivatives, this inner product can give a zero norm to nonzero functions. All one can deduce from knowing that $\int_{x_0}^{x_n} |g''(x)|^2\,dx = 0$ is that $g''(x) \equiv 0$, which does not imply that $f \equiv 0$ but rather that $f''(x) \equiv 0$ and thus that $f'(x) \equiv A$ and $f(x) \equiv Ax + B$ for some constants A, $B \in \mathbb{R}$. However, everything else we know about inner products will work pretty well with this one. In particular, we can see what really makes "Holladay's identity" go:

Sub-lemma: Let $\sigma(x) \in \mathcal{C}^2([a,b])$ satisfy the "Dirichlet(2) node conditions" $\sigma(x_i) = 0$ at all of the nodes $\{x_i : 0 \le i \le n\}$. Let $s(x)$ be any cubic spline with nodes at the $\{x_i\}$—that is, a function $s \in \mathcal{C}^2([a,b])$ whose restriction to each subinterval $J_i = [x_i, x_{i+1}]$ is a cubic polynomial. Then $\langle s, \sigma\rangle = 0$ under any of the following three additional hypotheses:

(1) $s(x)$ satisfies the "natural end conditions" $s''(x_0) = 0 = s''(x_n)$ (and no end conditions, other than taking the value zero, need be imposed on $\sigma(x)$);

(2) No end conditions are imposed on $s(x)$, but $\sigma(x)$ satisfies the "Neumann complete end conditions" $\sigma'(x_0) = 0 = \sigma'(x_n)$;

(3) $s(x)$ satisfies the "periodic end condition" $s''(x_0) = s''(x_n)$ and $\sigma(x)$ satisfies the "periodic end condition" $\sigma'(x_0) = \sigma'(x_n)$.

Proof. Consider the part of the integral $\langle s, \sigma\rangle = \int_{x_0}^{x_n} s''(x)\sigma''(x)\,dx$ over the interval $[x_i, x_{i+1}]$, and integrate by parts twice, letting "u" always be the derivative of s and "dv" always be the derivative of σ. One obtains

$$\begin{aligned}\int_{x_i}^{x_{i+1}} s''(x)\sigma''(x)\,dx &= s''(x)\sigma'(x)\Big]_{x_i}^{x_{i+1}} - \int_{x_i}^{x_{i+1}} s^{(3)}(x)\sigma'(x)\,dx \\ &= s''(x)\sigma'(x)\Big]_{x_i}^{x_{i+1}} - \left\{ s^{(3)}(x)\sigma(x)\Big]_{x_i}^{x_{i+1}} - \int_{x_i}^{x_{i+1}} s^{(4)}(x)\sigma(x)\,dx \right\} \\ &= s''(x)\sigma'(x)\Big]_{x_i}^{x_{i+1}} - s^{(3)}(x)\sigma(x)\Big]_{x_i}^{x_{i+1}} \quad \text{because } s^{(4)}(x) \equiv 0\ .\end{aligned}$$

Because $s''(x)$ is continuous on $[a,b]$—it "takes the same value from the left at each node x_i as it does from the right"—if we add these equations for $i = 0$ to $n-1$ the contributions from the first term on the last set-off line will "telescope." The contributions from the second term on that line will be zero, because $\sigma(x_i) = 0$ at all nodes. Therefore

$$\begin{aligned}\langle s, \sigma\rangle = \int_a^b s(x)\sigma(x)\,dx &= \sum_{i=0}^{n-1} [s''(x_{i+1})\sigma'(x_{i+1}) - s''(x_i)\sigma'(x_i)] \\ &= s''(b)\sigma'(b) - s''(a)\sigma'(a)\ .\end{aligned}$$

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(1) Strictly speaking, this is a "sesquilinear form" because it is conjugate-linear, rather than linear, in the argument g. However, we shall only deal with real-valued functions, so the complex-conjugation will really never have an effect.

(2) "Homogeneous boundary conditions"—requiring functions to take the value zero (possibly in some generalized sense) at the boundary of a region—traditionally bear the name *Dirichlet*.

In case (1), clearly $\langle s, \sigma \rangle = s''(b)\sigma'(b) - s''(a)\sigma'(a) = 0 - 0 = 0$, and similarly in case (2) where $\sigma'(a) = 0 = \sigma'(b)$. While it may not be the case that both terms of $s''(b)\sigma'(b) - s''(a)\sigma'(a)$ are zero in the third case, the terms will cancel if $s''(a) = s''(b)$ and $\sigma'(a) = \sigma'(b)$.

Proof of the lemma. Write $g = s - (s - g)$, let $\sigma(x)$ denote $s(x) - g(x)$, and observe that if $\langle s, \sigma \rangle = 0$ then we can write

$$\begin{aligned}\int_a^b |g''(x)|^2\, dx &= \langle g, g \rangle = \langle s, s \rangle - 2\langle s, \sigma \rangle + \langle \sigma, \sigma \rangle = \langle s, s \rangle + \langle \sigma, \sigma \rangle \\ &= \int_a^b |s''(x)|^2\, dx + \int_a^b |s''(x) - g''(x)|^2\, dx\end{aligned}$$

which is the conclusion of the lemma. If $s''(x)$ is a natural cubic spline interpolant of $f(x)$, then since $\sigma(x_i) = 0$ at all the nodes, we are in case (1) of the sublemma and $\langle s, \sigma \rangle = 0$. If $s(x)$ is a complete cubic spline interpolant of $f(x)$, then $\sigma(x) = s(x) - g(x)$ satisfies $\sigma'(x) = s'(x) - f'(x) = 0$ for $x = x_0$ and $x = x_n$, so we are in case (2) of the sublemma and $\langle s, \sigma \rangle = 0$. Finally, if $s(x)$ satisfies the end conditions $s'(x_0) = s'(x_n)$ and $s''(x_0) = s''(x_n)$ (as well as the interpolation condition $s(x_0) = f(x_0) = f(x_n) = s(x_n)$), then $\sigma'(x) = s'(x) - g'(x)$ takes equal values at x_0 and x_n also, so we are in case (3) of the sublemma and $\langle s, \sigma \rangle = 0$. Thus the conclusion of the lemma holds in all cases.

Corollary: The natural cubic spline interpolant of $f(x)$ (if it exists) minimizes $\int_a^b |g''(x)|^2\, dx$ over the class of *all* $\mathcal{C}^2$ interpolants $g(x)$ of $f(x)$ that equal $f(x)$ at all nodes. The complete cubic spline interpolant of $f(x)$ (if it exists) minimizes the same integral over the class of all $\mathcal{C}^2$ interpolants of $f(x)$ that equal $f(x)$ at all nodes and satisfy the endpoint conditions $g'(x_0) = f'(x_0)$ and $g'(x_n) = f'(x_n)$. Same for the periodic interpolant. In all these cases, the spline is the unique minimizing function.[3]

Proof. In all these cases, the appropriate case of Holladay's identity says

$$\int_a^b |g''(x)|^2\, dx = \int_a^b |s''(x)|^2\, dx + \int_a^b |s'' - g''|^2\, dx\ .$$

Evidently the r. h. s. is $\geq \int_a^b |s''|^2\, dx$, and equality will hold if and only if the continuous function $s''(x) - g''(x)$ is identically zero on $[a, b]$. So the integral of $|g''|^2$ must be *strictly* larger unless the $\mathcal{C}^2$ function $s(x) - g(x)$ satisfies the differential equation $y'' = 0$ on $[a, b]$. The solutions of that equation are the linear functions $y(x) = Ax + B$. In either case, since the function $s(x) - g(x) = Ax + B$ takes the value 0 both at $x = x_0$ and $x = x_n$ we must have $A = 0 = B$ and $s(x) - g(x) = 0$ identically, *i.e.*, $g(x)$ is identical to $s(x)$. We already saw minimization, and that's uniqueness.

We can use this uniqueness result to prove existence, although in a non-constructive way. The argument goes as follows. For a given function $f(x)$ there are $4n - 2$ equations in the coefficients of the polynomials $p_i(x)$ that must be satisfied in order for them, considered piecewise, to determine a cubic spline interpolant of $f(x)$:

$$\begin{aligned} f_i &= f(x_i), \quad i = 0, \ldots, n-1 \\ p_i(x_{i+1}) &= f(x_{i+1}), \quad i = 0, \ldots, n-1 \\ p_i'(x_{i+1}) - p_{i+1}'(x_{i+1}) &= 0, \quad i = 0, \ldots, n-2 \\ p_i''(x_{i+1}) - p_{i+1}''(x_{i+1}) &= 0, \quad i = 0, \ldots, n-2 \end{aligned}$$

and finally either the periodic endpoint conditions or

$$\begin{aligned} p_0''(x_0) &= 0 \quad \text{and} \quad p_{n-1}''(x_n) = 0 \quad \text{or} \\ p_0'(x_0) &= f'(x_0) \quad \text{and} \quad p_{n-1}'(x_n) = f'(x_n)\ . \end{aligned}$$

[3] The integral $\int_a^b |g''(x)|^2\, dx$ has a quasi-physical interpretation as "the energy required to bend a linearly elastic strip of metal into the curve that interpolates the function values." This proposition is consequently sometimes referred to as a "minimum-energy" characterization of cubic spline interpolants.

The interpolation conditions are inhomogeneous equations on the $\{f_i,\, b_i,\, c_i,\, d_i\}$; all the remaining conditions are homogeneous (r. h. s. zero) except for the complete-spline endpoint conditions. The total equation count is $4n$, and there are $4n$ unknown coefficients. By a well-known theorem on systems of linear equations, either every inhomogeneous case of these equations has a unique solution or else there exists a solution of the system

$$\begin{aligned} f_i &= 0, \quad i = 0, \ldots, n-1 \\ p_i(x_{i+1}) &= 0, \quad i = 0, \ldots, n-1 \\ p_i'(x_{i+1}) - p_{i+1}'(x_{i+1}) &= 0, \quad i = 0, \ldots, n-2 \\ p_i''(x_{i+1}) - p_{i+1}''(x_{i+1}) &= 0, \quad i = 0, \ldots, n-2 \end{aligned}$$

and finally either

$$\begin{aligned} p_0''(x_0) = 0 \quad &\text{and} \quad p_{n-1}''(x_n) = 0 \quad \text{or} \\ p_0'(x_0) = 0 \quad &\text{and} \quad p_{n-1}'(x_n) = 0 \end{aligned}$$

or the periodic endpoint conditions hold (depending on the case considered), in which not all of the numbers $\{f_i,\, b_i,\, c_i,\, d_i\}$ equal zero. Now suppose the latter case could actually occur—that there were a solution of these homogeneous equations. The resulting function $s(x)$ defined by the $p_i(x)$'s would indeed be $\mathcal{C}^2$, and it would be a complete, natural or periodic spline interpolant of the function $f(x)$ which is identically zero. But $f(x)$ identically zero also satisfies the defining conditions to be such a spline interpolant of itself. By uniqueness of the spline interpolant, $s(x) = 0$ identically. But then each $p_i(x) = 0$ identically, so all its coefficients are zero, so all the $\{f_i,\, b_i,\, c_i,\, d_i\}$ are zero contrary to their choice! We conclude that the equations which must be solved to find the coefficients of the polynomials making up a spline interpolant are determined by $4n$ equations in $4n$ unknowns where the equations have no nontrivial homogeneous solutions; the equations are therefore uniquely solvable for any choice of r. h. s.'s, and so they can always be solved to yield the coefficients of the polynomials in the cubic spline interpolant of any given $f(x)$. This establishes the existence of cubic spline interpolants (we already had uniqueness).

We shall give an algorithm for finding the coefficients later on. Meanwhile, it is nice to know that one is talking about things that actually exist when one proves theorems about cubic spline interpolants.

5. Setting up the equations. Determining the $\{b_i\}$ is actually most easily done by writing the polynomials in Newton form and solving the following Hermite interpolation problem (the b_i are not yet known and are to be determined)

$$p_i(x_i) = f_i,\ p_i'(x_i) = b_i,\ p_i(x_{i+1}) = f_{i+1},\ p_i'(x_{i+1}) = b_{i+1}\ .$$

Newton interpolation then gives us $p_i(x)$ as

$$p_i(x) = f_i + p_i[x_i, x_i](x - x_i) + p_i[x_i, x_i, x_{i+1}](x - x_i)^2 + p_i[x_i, x_i, x_{i+1}, x_{i+1}](x - x_i)^2(x - x_{i+1})$$

and the divided differences are explicitly computed in terms of the values of f_i, f_{i+1}, b_i, b_{i+1} and $f[x_i, x_{i+1}]$ in the first divided-difference table of Table 1.

To get this into Taylor form is easy: rewrite the single factor $(x - x_{i+1})$ in the form

$$x - x_{i+1} = x - x_i + x_i - x_{i+1} = (x - x_i) - h_i$$

and the Newton form turns into the Taylor form

$$\begin{aligned} p_i(x) = f_i &+ p_i[x_i, x_i](x - x_i) \\ &+ \{p_i[x_i, x_i, x_{i+1}] - h_i \cdot p_i[x_i, x_i, x_{i+1}, x_{i+1}]\}(x - x_i)^2 \\ &+ p_i[x_i, x_i, x_{i+1}, x_{i+1}](x - x_i)^3\ . \end{aligned}$$

These calculations find $p_i(x)$ "looking right from x_i." On the other hand, "looking left from x_i" almost the same calculations would have done the interpolation problem to find $p_{i-1}(x)$, because cubic Hermite

Table 1

Looking right from x_i:

x	$f(x_k)$	$p_i[\cdot,\cdot]$	$p_i[\cdot,\cdot,\cdot]$	$p_i[\cdot,\cdot,\cdot,\cdot]$
x_i	f_i	b_i	$\dfrac{f[x_i,x_{i+1}]-b_i}{h_i}$	$\dfrac{b_i+b_{i+1}-2f[x_i,x_{i+1}]}{h_i^2}$
x_i	f_i	$f[x_i,x_{i+1}]$	$\dfrac{b_{i+1}-f[x_i,x_{i+1}]}{h_i}$	
x_{i+1}	f_{i+1}	b_{i+1}		
x_{i+1}	f_{i+1}			

Looking left from x_i:

x	$f(x_k)$	$p_{i-1}[\cdot,\cdot]$	$p_{i-1}[\cdot,\cdot,\cdot]$	$p_{i-1}[\cdot,\cdot,\cdot,\cdot]$
x_i	f_i	b_i	$\dfrac{f[x_{i-1},x_i]-b_i}{-h_{i-1}}$	$\dfrac{b_{i-1}+b_i-2f[x_{i-1},x_i]}{h_{i-1}^2}$
x_i	f_i	$f[x_{i-1},x_i]$	$\dfrac{b_{i-1}-f[x_{i-1},x_i]}{-h_{i-1}}$	
x_{i-1}	f_{i-1}	b_{i-1}		
x_{i-1}	f_{i-1}			

---

interpolation imposes two conditions at each node and thus the problem of determining $p_{i-1}(x)$ at x_i is symmetric to that of determining $p_i(x)$ there. In Newton form, $p_{i-1}(x)$ must be

$$\begin{aligned}p_{i-1}(x) = f_i &+ p_{i-1}[x_i,x_i](x-x_i)\\ &+ p_{i-1}[x_i,x_i,x_{i-1}](x-x_i)^2\\ &+ p_{i-1}[x_i,x_i,x_{i-1},x_{i-1}](x-x_i)^2(x-x_{i-1})\ .\end{aligned}$$

Again the Newton form can be put into Taylor form with base-point x_i by rewriting

$$x-x_{i-1} = x-x_i+x_i-x_{i-1} = (x-x_i)+h_{i-1}$$

and so the Taylor form of $p_{i-1}(x)$ at x_i is

$$\begin{aligned}p_{i-1}(x) = f_i &+ p_{i-1}[x_i,x_i](x-x_i)\\ &+ \{p_{i-1}[x_i,x_i,x_{i-1}] + h_{i-1}\cdot p_{i-1}[x_i,x_i,x_{i-1},x_{i-1}]\}(x-x_i)^2\\ &+ p_{i-1}[x_i,x_i,x_{i-1},x_{i-1}](x-x_i)^3\ .\end{aligned}$$

Since these polynomials are in Taylor form with base point x_i, one can read their derivatives at x_i right off their Taylor coefficients. That the 0-th and 1st Taylor coefficients are equal simply expresses the facts that both polynomials take the value f_i and that both have derivative b_i at that point. The coefficients of $(x-x_i)^2$, however, are the second derivatives of the polynomials up to a factor of 2!. Hence a necessary and sufficient condition for the polynomials to have equal second derivatives at the break point x_i is that

$$p_i[x_i,x_i,x_{i+1}] - h_i\cdot p_i[x_i,x_i,x_{i+1},x_{i+1}] = p_{i-1}[x_i,x_i,x_{i-1}] + h_{i-1}\cdot p_{i-1}[x_i,x_i,x_{i-1},x_{i-1}]$$

which Table 1 tells us is

$$\frac{f[x_i,x_{i+1}]-b_i}{h_i} - h_i\cdot\frac{b_i+b_{i+1}-2\cdot f[x_i,x_{i+1}]}{h_i^2} = \frac{f[x_i,x_{i-1}]-b_i}{-h_{i-1}} + h_{i-1}\cdot\frac{b_{i-1}+b_i-2\cdot f[x_i,x_{i-1}]}{h_{i-1}^2}$$

in terms of known quantities. With both sides multiplied by $h_i \cdot h_{i-1}$ this is

$$h_{i-1} \cdot \{f[x_i, x_{i+1}] - b_i\} - h_{i-1} \cdot \{b_i + b_{i+1} - 2 \cdot f[x_i, x_{i+1}]\} = h_i \cdot \{b_i - f[x_i, x_{i-1}]\} + h_i \cdot \{b_{i-1} + b_i - 2 \cdot f[x_i, x_{i-1}]\}$$

and this, with the unknown b_i's kept on the r. h. s. and the known quantities moved to the l. h. s., becomes an equation

$$3 \cdot h_i \cdot f[x_i, x_{i-1}] + h_{i-1} \cdot f[x_i, x_{i+1}] = h_i \cdot b_{i-1} + (h_{i-1} + h_i) \cdot 2b_i + h_{i-1} \cdot b_{i+1}$$

that is to be satisfied at each of the interior nodes, $i = 1, \ldots, n-1$. One more piece of beautification and we'll have something that's worth trying to solve: divide the i-th equation by $(h_{i-1} + h_i)$ and put

$$\mu_i = \frac{h_i}{h_{i-1} + h_i}, \qquad \lambda_i = \frac{h_{i-1}}{h_{i-1} + h_i} .$$

These are "convex combination coefficients"—pairs of nonnegative numbers satisfying $\mu_i + \lambda_i = 1$—and with the unknown b_i's on the l. h. s. where unknowns belong, the equations determining the b_i's take the form

$$\mu_i b_{i-1} + 2b_i + \lambda_i b_{i+1} = 3 \cdot \{\mu_i f[x_i, x_{i-1}] + \lambda_i f[x_i, x_{i+1}]\}$$

for $i = 1, \ldots, n-1$. We need two more equations, and we take those to be

$$\begin{aligned} 2b_0 &= 2b_0 \qquad (= 2f'(x_0)) \\ 2b_n &= 2b_n \qquad (= 2f'(x_n)) \end{aligned}$$

which is to say that we shall be finding the coefficients in the **complete cubic spline interpolant** of $f(x)$. The factors of 2 are present only for the sake of symmetry of notation.

The equations determining the b_i's then take the form

$$\begin{array}{lllllcl}
2b_0 & & & & \cdots\ \cdots & = & 2f'(x_0) \\
& \mu_1 b_0 + 2b_1 + \lambda_1 b_2 & & & \cdots\ \cdots & = & 3 \cdot \{\mu_1 f[x_1, x_0] + \lambda_1 f[x_1, x_2]\} \\
& & \mu_2 b_1 + 2b_2 + \lambda_2 b_3 & & \cdots\ \cdots & = & 3 \cdot \{\mu_2 f[x_2, x_1] + \lambda_2 f[x_2, x_3]\} \\
\cdots & \cdots & \cdots & \ddots & \cdots\ \cdots & \vdots & \cdots \\
& & & & 2b_n & = & 2f'(x_n)
\end{array}$$

and are $(n+1)$ linear equations in the $(n+1)$ unknowns $(b_0, \ldots, b_n)$.

6. The R. H. Sides of the equations we have just derived are fairly easy to compute and to estimate in terms of $f'(x)$ (when it exists); indeed, it should be obvious to the reader that each can only be about 3 times(4) as large as any value of $f'(x)$. But we don't yet know that the equations can be solved at all, or that $(b_0, \ldots, b_n)^T$ will not exhibit unpleasant behavior. It is therefore a marvelous piece of luck that these equations belong to one of the most tractable classes of linear systems: those whose matrix of coefficients is **strictly diagonally dominant**.(5) Since we don't need the most general properties of these systems, the following lemma is enough to give us what we need now. To accomodate ancient habits we'll write the system in the form $AX = Y$, where X and Y are vectors, for the duration of this § only. Let us agree that the **norm** of a vector $X = (x_0, \ldots, x_n)^T$ will be the ℓ^∞-norm, *i.e.*, will be given by

$$\|X\|_\infty = \max\{|x_i| : i = 0, \ldots, n\} .$$

(4) In fact, if we further "normalized" these equations by dividing the top and bottom ones by 2 and the others by 3, we would see that what these equations do is balance weighted averages of the b_i's on the l. h. sides against weighted averages of values (at nearby points) of $f'(x)$ on the r. h. sides.

(5) See the separate notes on systems of this kind for a more complete discussion of these matrices than is given here.

Lemma: Let $AX = Y$ be an $(n+1) \times (n+1)$ system of linear equations whose matrix of coefficients has the "tri-diagonal" form

$$\begin{bmatrix} 2 & \lambda_0 & 0 & 0 & \cdots & 0 & 0 \\ \mu_1 & 2 & \lambda_1 & 0 & \cdots & 0 & 0 \\ 0 & \mu_2 & 2 & \lambda_2 & \cdots & 0 & 0 \\ 0 & 0 & \mu_3 & 2 & \cdots & 0 & 0 \\ 0 & \vdots & \vdots & \vdots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 2 & \lambda_{n-1} \\ 0 & 0 & 0 & 0 & \cdots & \mu_n & 2 \end{bmatrix}$$

where[(6)] the off-diagonal coefficients satisfy $|\mu_i| + |\lambda_i| \le 1$. Then for any given pair of vectors X, Y satisfying the equations, we have $\|X\|_\infty \le |y_k|$, where $0 \le k \le n$ is any index[(7)] at which the maximum defining $\|X\|_\infty = \max\{|x_i| : i = 0, \ldots, n\}$ is attained. In particular,

$$\|X\|_\infty \le \|Y\|_\infty \,.$$

Proof. Let X and Y be such vectors and A be such a matrix, and let the index k be as described. Then (the appropriate terms being missing in the cases $k = 0$ and $k = n$) we have

$$\begin{aligned} \mu_k x_{k-1} + 2x_k + \lambda_k x_{k+1} &= y_k \\ 2x_k &= y_k - \mu_k x_{k-1} - \lambda_k x_{k+1} \,. \end{aligned}$$

Taking absolute values and using the triangle inequality, we get

$$\begin{aligned} 2|x_k| &\le |y_k| + |\mu_k||x_{k-1}| + |\lambda_k||x_{k+1}| \le |y_k| + |\mu_k||x_k| + |\lambda_k||x_k| \\ &= |y_k| + (|\mu_k| + |\lambda_k|)|x_k| \le |y_k| + |x_k| \,. \end{aligned}$$

Finally, subtracting $|x_k|$ from both sides gives us

$$\|X\|_\infty = |x_k| \le |y_k| \le \|Y\|_\infty$$

as desired.

Corollary: $AX = Y$ has a unique solution X for every given Y (and that solution must satisfy the norm inequality $\|X\|_\infty \le \|Y\|_\infty$).

Proof. Any solution of $AX = 0$ satisfies $\|X\|_\infty \le \|0\|_\infty$, so $X = 0$. Thus the associated homogeneous $(n+1) \times (n+1)$ system $AX = 0$ has only the trivial (all-zero) solution. It is a standard theorem of linear algebra that this property implies that $AX = Y$ is solvable (and uniquely so) for each given Y.

{Remark: That corollary was proved unconstructively, but these matrices have a computational property that enables one to show that the system $AX = Y$ can always be solved by Gaussian elimination without pivoting. And the Gaussian elimination is trivial: in each column there is only one sub-diagonal element. Thus machine solution of such "tridiagonal diagonally dominant" systems is very fast compared to systems in general. See the separate notes on diagonally dominant matrices, in which it is shown that the "strict diagonal dominance" condition $|a_{ii}| > \sum_{j \ne i} |a_{ij}|$ is preserved as the Gaussian elimination algorithm progresses. Strict diagonal dominance implies invertibility, by the Geršgorin theorem.}

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(6) This lemma is basically a very special case of the general Geršgorin theorem on locating the eigenvalues of a matrix—and estimating the norm of its inverse—in terms of the diagonal elements of the matrix.

(7) This is a "discrete maximum principle," much like the maximum principle of potential theory.

7. Approximation by an Interpolating Spline. Even when the interpoland $f(x)$ is only $\mathcal{C}^2$, it turns out that the spline interpolants approximate $f(x)$ *and* their derivatives approximate $f'(x)$ quite well, uniformly on J. For smoother interpolands, the approximations are good out to $f^{(3)}(x)$.

For the $\mathcal{C}^2$ case, the estimate employs the "minimum-energy" characterization of the cubic spline interpolants, and the estimates are not of the order of magnitude in h that one will learn to expect for smoother functions. The basic tool is the Schwarz inequality for integrals, which asserts that for two (Lebesgue-measurable) real-valued functions f and g on an interval $[\alpha, \beta]$, the inequality

$$\int_\alpha^\beta |f(x)g(x)|\,dx \le \sqrt{\int_\alpha^\beta f(x)^2\,dx} \cdot \sqrt{\int_\alpha^\beta g(x)^2\,dx}$$

always holds. For a proof, see the **Lemma** of Atkinson p. 208.

Theorem: Let $f(x)$ be a $\mathcal{C}^2$ function[8] on J and $s(x)$ a cubic spline interpolant of f. Then the estimate

$$|f'(x) - s'(x)| \le h^{1/2} \cdot \sqrt{\int_a^b |f''(t)|^2\,dt}$$

holds (uniformly) for all $x \in J$.

Proof. Let $x \in J$ be given, and let $[x_i, x_{i+1}]$ be a cell to which it belongs. Then since $f(t) - s(t) = 0$ for $t = x_i$ and $t = x_{i+1}$, by Rolle's theorem there exists $\xi \in [x_i, x_{i+1}]$ for which $f'(\xi) - s'(\xi) = 0$. We therefore have in the case where $\xi < x$—and the same argument, with the direction of integration reversed, covers the case $x < \xi$:

$$\begin{aligned} |f'(x) - s'(x)| = \left| \int_\xi^x [f''(t) - s''(t)]\,dt \right| &\le \sqrt{\int_\xi^x 1\,dt} \cdot \sqrt{\int_\xi^x [f''(t) - s''(t)]^2\,dt} \\ &\le |x - \xi|^{1/2} \cdot \sqrt{\int_a^b [f''(t) - s''(t)]^2\,dt}\,. \end{aligned}$$

In the last line, we evaluated the integral of 1 over $[\xi, x]$ and replaced the integral of the square-of-the-difference of 2nd derivatives over $[\xi, x]$ by the integral over the whole $[x_0, x_n]$, which could only have made the integral bigger. But now we can estimate both factors in the last line: it is obvious that $|x - \xi|^{1/2} \le h^{1/2}$, while if we replace g'' by f'' in Holladay's identity on pp. 4–5 above we see that the nonnegativity of the integral of s''^2 then implies

$$\int_a^b |f''(t)|^2\,dt \ge \int_a^b |s''(t) - f''(t)|^2\,dt\,.$$

Using those estimates in the relation above then gives us

$$|f'(x) - s'(x)| \le h^{1/2} \cdot \sqrt{\int_a^b |f''(t)|^2\,dt]};,$$

as desired.

Corollary: The estimate

$$|f(x) - s(x)| \le \frac{1}{2}\,h^{3/2} \cdot \sqrt{\int_a^b |f''(t)|^2\,dt}$$

holds (uniformly) for all $x \in J$.

(8) It would suffice for this that $f(x)$ belong to the Sobolëv space $W^{2,2}(J)$, which would imply that it had a continuous first derivative but only that it had a second derivative in the "weak" or "distributional" sense that belonged to $L^2(J)$. The fact that one can assume only this rather shadowy existence for the second derivative is the reason for the low order of approximation.

Proof. Let $x \in J$ be given, and let $[x_i, x_{i+1}]$ be a cell to which it belongs. Then since $f(t) - s(t) = 0$ for $t = x_i$ and $t = x_{i+1}$, we can compute $f(x) - s(x)$ {up to its sign} by integrating $f'(t) - s'(t)$ from the nearer endpoint of $[x_i, x_{i+1}]$—call it x^*—to x:

$$|f(x) - s(x)| = \left| \int_{x^*}^{x} (f'(t) - s'(t))\, dt \right| \leq \max\{|x - x^*|\} \cdot \max\{|f'(t) - s'(t)| : t \in J\}$$

$$\leq \frac{1}{2}\, h \cdot h^{1/2} \cdot \sqrt{\int_a^b |f''(t)|^2\, dt} = \frac{1}{2}\, h^{3/2} \cdot \sqrt{\int_a^b |f''(t)|^2\, dt}$$

as advertised.

These are "modern" estimates—estimates of this type will recur at the end of the second second-semester course, when one develops the finite-element method of solving boundary-value problems in differential equations. However, they're not very sharp: the exponents in $h^{3/2}$ and $h^{1/2}$ really "should" be 4 and 3 respectively, at least when $f(x)$ is a sufficiently smooth function. Developing estimates of that order requires a great deal of classical technique, and we shall demonstrate that technique in the next §. Meanwhile, even the coarse estimates available from the "energy integral" show that as $h \to 0$ we can expect cubic spline interpolants of $\mathcal{C}^2$ functions to converge to the interpoland—and, even better, the derivatives converge also {although "one power of h more slowly"}. That fact at least reassures us that the cubic spline interpolant is a reasonable subject of investigation.

8. Classical Error Estimates for Cubic Splines. We can now start to estimate the difference between the given function $f(x)$ and its complete cubic spline interpolant in the classical way, with bounds involving the maximum absolute values of the higher derivatives of $f(x)$. This is time-consuming but each step is elementary. We shall carry out the steps in the following order:

(A) Working locally (for x in a single cell $[x_i, x_{i+1}]$) we can rewrite the difference between $f(x)$ and $p_i(x)$ in the form

$$f(x) - p_i(x) = f(x) - H(x) + H(x) - p_i(x)$$

where $H(x)$ is the cubic Hermite interpolant of $f(x)$ (and $f'(x)$) on $[x_i, x_{i+1}]$, use the triangle inequality

$$|f(x) - p_i(x)| \leq |f(x) - H(x)| + |H(x) - p_i(x)|\ ,$$

and estimate the two terms separately. The first term is the error term from Hermite interpolation, for which bounds are known (Atkinson p. 162, (3.6.15)).

(B) That leaves the second error term

$$e_i(x) = p_i(x) - H(x)$$

which is a polynomial of degree ≤ 3 satisfying

$$e_i(x_i) = 0 = e_i(x_{i+1}),\ e_i'(x_i) = b_i - f'(x_i),\ e_i'(x_{i+1}) = b_{i+1} - f'(x_{i+1})\ .$$

If we set

$$\epsilon_i = e_i'(x_i) = b_i - f'(x_i) \quad \text{and} \quad \epsilon_{i+1} = e_i'(x_{i+1}) = b_{i+1} - f'(x_{i+1})\ ,$$

then e_i can easily be estimated in terms of $\max\{|\epsilon_i|, |\epsilon_{i+1}|\}$. It is clear from these definitions that $\epsilon_0 = 0$, and the only consistent definition of ϵ_n is to set it $= 0$ also.

(C) The $(n+1)$-tuple $(0, \epsilon_1, \ldots, \epsilon_{n-1}, 0)^T$ satisfies a system of $(n+1)$ linear equations of the form $AX = Y$ with the same matrix of coefficients A as the system that determined $(b_0, b_1, \ldots, b_n)^T$. The r. h. s. of that system can be written out explicitly and its elements estimated. Because $AX = Y$ implies $\|X\|_\infty \leq \|Y\|_\infty$, the estimate thus obtained also controls $\max\{|\epsilon_0|, \ldots, |\epsilon_n|\}$; using the result of part **(B)** above, we then make that estimate control the error cubics $e_i(x)$ $(i = 0, \ldots, n-1)$, thus finishing the estimation process for the complete cubic spline interpolant.

(D) The error in the natural cubic spline interpolant, and the errors in the cubic splines produced by other possible choices of endpoint conditions, are most easily handled by estimating the errors between those interpolants and the complete interpolant.

Hypotheses will be introduced naturally along the way: usually they will require that $f(x)$ have 4 or 5 continuous derivatives on J. For future reference we recall the standard notation

$$M_k = \max\{|f^{(k)}(x)| : x_0 \le x \le x_n\}$$

for all functions $f(x)$ for which this expression makes sense. Recall also that

$$h = \max\{h_0, \ldots, h_n\} .$$

9. Estimate (A). Not much to do here: Atkinson's (3.6.13) gives

$$|f(x) - H(x)| \le \frac{h^4}{384} \cdot M_4$$

which is sharp (take $f(x) = x^4$).

10. Estimate (B). The error cubic $e_i(x)$ is a polynomial whose degree is at most 3, and it has a root at each end of $[x_i, x_{i+1}]$, so it must have the form

$$e_i(x) = (x - x_i)(x - x_{i+1})[a(x - x_i) + b] .$$

Its derivative thus has the form

$$e_i'(x) = (x - x_{i+1})[a(x - x_i) + b] + (x - x_i)[a(x - x_i) + b] + a(x - x_i)(x - x_{i+1}) ,$$

and evaluation, first at x_i and then at x_{i+1}, shows that the linear function in the square brackets has to interpolate the values

$$\frac{\epsilon_i}{-h_i} \;\text{ at }\; x = x_i \quad\text{and}\quad \frac{\epsilon_{i+1}}{h_i} \;\text{ at }\; x = x_{i+1} .$$

Therefore this linear factor is $\dfrac{\epsilon_{i+1}(x - x_i) - \epsilon_i(x_{i+1} - x)}{h_i^2}$, and so

$$e_i(x) = (x - x_i)(x - x_{i+1})\,\frac{\epsilon_{i+1}(x - x_i) - \epsilon_i(x_{i+1} - x)}{h_i^2} .$$

The product $|(x-x_i)(x-x_{i+1})|$ assumes its maximum at the midpoint of the cell $[x_i, x_{i+1}]$, and the maximum value is $(h/2)^2$. The linear factor assumes its maximum value at an endpoint, so its maximum value can be estimated by $\dfrac{\max\{|\epsilon_i|, |\epsilon_{i+1}|\}}{h_i}$. This gives the estimate

$$|e_i(x)| \le \frac{h_i^2}{4} \cdot \frac{\max\{|\epsilon_i|, |\epsilon_{i+1}|\}}{h_i} = \frac{h_i}{4} \cdot \max\{|\epsilon_i|, |\epsilon_{i+1}|\} .$$

We can do no better than this in general, since we may have $\epsilon_i = -\epsilon_{i+1}$ and then the linear factor will reduce to a constant.

11. Estimate (C). Since we have defined

$$\epsilon_i = e_i'(x_i) = b_i - f'(x_i) \quad\text{and}\quad \epsilon_{i+1} = e_i'(x_{i+1}) = b_{i+1} - f'(x_{i+1})$$

the equations defining the b_i's that come from the interior nodes

$$\mu_i b_{i-1} + 2b_i + \lambda_i b_{i+1} = 3 \cdot \{\mu_i f[x_i, x_{i-1}] + \lambda_i f[x_i, x_{i+1}]\}$$

can be rewritten in the form (note that we have used $1 = \mu_i + \lambda_i$)

$$\mu_i\epsilon_{i-1}+2\epsilon_i+\lambda_i\epsilon_{i+1} = \mu_i\cdot\{3f[x_i,x_{i-1}]-f'(x_{i-1})-2f'(x_i)\}+\lambda_i\cdot\{3f[x_i,x_{i+1}]-f'(x_{i+1})-2f'(x_i)\} \quad (11.1)$$

for $i = 1, \ldots, n-1$, and of course at the endpoints we simply have

$$\epsilon_0 = 0, \quad \epsilon_n = 0$$

since the derivative of the spline matches the derivative of $f(x)$ at the endpoints. Because of what we know about the matrix of coefficients of this system of equations, we know that if we find a bound for the absolute values of all the r. h. sides of these equations, the same bound will dominate the absolute values of all the ϵ_i's. The first thing on the agenda, therefore, is to find a sharp bound for those r. h. sides.

One method of attack is to rewrite the differences on the r. h. sides as integrals. This method recurs again and again in error analysis, and so it will pay us to write it up in as general a way as possible. Thus let $F(t)$ be a 5-times-continuously differentiable function defined on an open interval $-\eta < t < \eta$ centered on 0, let $|h| < \eta$, and consider

$$3\cdot F[0,h]-F'(h)-2\cdot F'(0) = \frac{1}{h}\int_0^h \{[F'(t)-F'(h)]+2\cdot[F'(t)-F'(0)]\}\,dt\ . \quad (11.2)$$

Integrate the term $[F'(t)-F'(h)]\,dt$ by parts, differentiating the first factor and using as the integral of dt the function t, which takes the value zero at the endpoint 0. Similarly integrate the term $2[F'(t)-F'(0)]\,dt$ by parts, differentiating the first factor but this time using as the integral of dt the function $(t-h)$ which zeros out at the endpoint h. The result will be that the integral is rewritten as

$$\frac{-1}{h}\int_0^h \{t+2(t-h)\}\cdot F''(t)\,dt = \frac{-3}{h}\int_0^h \left(t-\frac{2}{3}h\right)F''(t)\,dt\ . \quad (11.3)$$

Next, express $F''(t)$ in a Taylor series with base point $t = 0$, writing the remainder term in integral form:

$$F''(t) = F''(0)+F^{(3)}(0)\cdot t+\int_0^h (t-s)F^{(4)}(s)\,ds\ . \quad (11.4)$$

Plugging this in for $F''(t)$ in the previous integral will show that our original $3\cdot F[0,h]-F'(h)-2\cdot F'(0)$ equals

$$\frac{-3}{h}\int_0^h \left(t-\frac{2}{3}h\right)\left\{F''(0)+t\cdot F^{(3)}(0)+\int_0^t (t-s)F^{(4)}(s)\,ds\right\}\,dt\ . \quad (11.5)$$

It is elementary to multiply the first two terms inside the curly brackets by $(t-(2h)/3)$ and integrate the results, obtaining the values $\dfrac{-h^2}{6}F''(0)$ and 0 respectively. If these values are plugged in and the order of integration in the double integral is then reversed, the whole expression becomes

$$\frac{-3}{h}\left\{\frac{-h^2}{6}F''(0)+\int_0^h\left[\int_s^h\left(t-\frac{2}{3}h\right)(t-s)\,dt\right]F^{(4)}(s)\,ds\right\}\ . \quad (11.6)$$

It is routine to evaluate the inside integral; its value is $\dfrac{s(h-s)^2}{6}$. So we finally have

$$3\cdot F[0,h]-F'(0)-2\cdot F'(h) = \frac{-1}{h}\left\{\frac{-h^2}{2}F''(0)+\frac{1}{2}\int_0^h s(h-s)^2F^{(4)}(s)\,ds\right\}\ . \quad (11.7)$$

One should note for future reference that the sign of the factor $s(h-s)^2$ in the "remainder term" is the same as the sign of h.

At this point we are ready to attack the r. h. s. of the equation (11.1)

$$\mu_i\epsilon_{i-1} + 2\epsilon_i + \lambda_i\epsilon_{i+1} = \mu_i \cdot \{3f[x_i, x_{i-1}] - f'(x_{i-1}) - 2f'(x_i)\} + \lambda_i \cdot \{3f[x_i, x_{i+1}] - f'(x_{i+1}) - 2f'(x_i)\}\ .$$

Both expressions in the curly brackets have the form $3 \cdot F[0, h] - F'(h) - 2 \cdot F'(0)$ with $F(t) = f(x_i + t)$, $h = -h_{i-1}$ in the first and $F(t) = f(x_i + t)$, $h = h_i$ in the second. Recalling that $\mu_i = \dfrac{h_i}{h_{i-1} + h_i}$ and $\lambda_i = \dfrac{h_{i-1}}{h_{i-1} + h_i}$, we can rewrite the whole r. h. side of (11.1) by using (11.7). The reader can easily check that the two terms containing the factor $F''(0) = f''(x_i)$ cancel, and the r. h. s. takes the form (watch signs!)

$$\frac{1}{h_{i-1} + h_i}\Bigg\{h_i \cdot \frac{-1}{-h_{i-1}}\left[\frac{-h_{i-1}^2}{2} f''(x_i) + \frac{1}{2}\int_0^{-h_{i-1}} s(-h_{i-1} - s)^2 f^{(4)}(x_i + s)\, ds\right]$$
$$+h_{i-1} \cdot \frac{-1}{h_i}\left[\frac{-h_i^2}{2} f''(x_i) + \frac{1}{2}\int_0^{h_i} s(h_i - s)^2 f^{(4)}(x_i + s)\, ds\right]\Bigg\} =$$
$$\frac{-1}{2(h_{i-1} + h_i)}\left\{\frac{h_i}{h_{i-1}}\int_{-h_{i-1}}^0 s(h_{i+1} + s)^2 f^{(4)}(x_i + s)\, ds + \frac{h_{i-1}}{h_i}\int_0^{h_i} s(h_i - s)^2 f^{(4)}(x_i + s)\, ds\right\}\ . \qquad (11.8)$$

A well-known mean-value theorem for integrals says that when $m \le f(s) \le M$ and $g(s) \ge 0$, then for $\alpha < \beta$

$$m\int_\alpha^\beta g(s)\, ds \le \int_\alpha^\beta f(s)g(s)\, ds \le M\int_\alpha^\beta g(s)\, ds\ .$$

It follows (let $g(s) = s(h_{i-1} + s)^2$ in the first integral, for example) that each of the the two integrals in the curly brackets can be estimated in absolute value by $\dfrac{h_i}{h_{i-1}} \cdot \dfrac{h_{i-1}^4}{12} \cdot M_4$ and $\dfrac{h_{i-1}}{h_i} \cdot \dfrac{h_i^4}{12} \cdot M_4$ respectively. So the entire r. h. side is now estimated in absolute value by the expression

$$\frac{1}{24} \cdot \frac{h_{i-1}h_i}{h_{i-1} + h_i} \cdot (h_{i-1}^2 + h_i^2) \cdot M_4\ . \qquad (11.9)$$

Finding the maximum value of the factor involving the h_i's is essentially the calculus problem of maximizing $\dfrac{xy(x^2 + y^2)}{x + y}$ on the square $0 \le x \le h$, $0 \le y \le h$. If this problem is subjected to the additional constraint that $x + y = a$, then one is looking for the maximum of $\dfrac{x(a - x)[x^2 + (a - x)^2]}{a}$, which occurs when $x = a/2$ (the derivative is $\dfrac{(a - 2x)^3}{a}$), *i.e.*, on the center-line $x = y$. Since $x = y = h$ is possible, the maximum value is h^3. We have thus shown that the r. h. s. is majorized in absolute value by $\dfrac{h^3}{24} \cdot M_4$.

We have just estimated the r. h. s. of an equation of the system (11.1)

$$\mu_i\epsilon_{i-1} + 2\epsilon_i + \lambda_i\epsilon_{i+1} = \mu_i \cdot \{3f[x_i, x_{i-1}] - f'(x_{i-1}) - 2f'(x_i)\} + \lambda_i \cdot \{3f[x_i, x_{i+1}] - f'(x_{i+1}) - 2f'(x_i)\}\ ,$$

but since $1 \le i \le n - 1$ was arbitrary and $\epsilon_0 = \epsilon_n = 0$, we have estimated the $\|\cdot\|_\infty$-norm of the vector r. h. s. $(\epsilon_0, \ldots, \epsilon_{n-1})^T$ of the system. By the "norm-reducing" property of the system, we can now conclude that

$$\max\{|\epsilon_i| : 0 \le i \le n\} \le \frac{h^3}{24} \cdot M_4 \qquad (11.10)$$

and thus we have come to the end-game of **(C)**: since **(B)** above now allows us to write

$$\max\{|e_i(x)| : x_i \le x \le x_{i+1}\} \le \frac{h}{4} \cdot \max\{|\epsilon_i| : 0 \le i \le n\} \le \frac{h}{4} \cdot \frac{h^3}{24} \cdot M_4 = \frac{h^4}{96} \cdot M_4\ , \qquad (11.11)$$

we can conclude that

$$|f(x) - p_i(x)| \le |f(x) - H(x)| + |e_i(x)| \le \frac{h^4}{384} \cdot M_4 + \frac{h^4}{96} \cdot M_4 = \frac{5h^4}{384} \cdot M_4 \tag{11.12}$$

and that estimates the error of the complete cubic spline interpolant, as desired.

In order to make a worst-case estimate of the integrals above by the mean-value theorem, we had to act as if it were possible for $f^{(4)}(x)$ to equal $+1$ on one side of x_i and -1 on the other side. While in fact $f^{(4)}(x)$ cannot do this if it is continuous, it is possible to find (draw pictures!) functions whose behavior is arbitrarily close to that, so no improvement in the estimate of the $\{|\epsilon_i|\}$ is possible. The function $x^4 \cdot \text{sgn}(x)$ has that impossible 4-th derivative, and its spline interpolant (Fig. 1) demonstrates that the slope of the interpolant can differ a good deal from that of the curve at a node. In the plot shown in Fig. 1 we have $x_0 = -1$, $x_1 = 0$, $x_2 = 1$. This function is a limiting case of 4-times continuously differentiable functions, so they can be "arbitrarily close to this bad."

12. Refinements. It can be shown that the constant 5/384 of the preceding § is the best possible constant valid for arbitrary 4-times differentiable $f(x)$ and arbitrary nodes whose maximum spacing is $h > 0$. However, some improvements are possible in the case of equal increments (all $h_i = h$). In this case, and assuming that the function $F(x)$ is 5-times continuously differentiable, we can replace $F^{(4)}(s)$ in the formula (11.7) above by

$$F^{(4)}(0) + \int_0^s F^{(5)}(t)\, dt\ , \tag{12.1}$$

whereupon (11.7) will read

$$\frac{-1}{h}\left\{\frac{-h^2}{2} F''(0) + \frac{1}{2}\int_0^t s(h-s)^2 \left[F^{(4)}(0) + \int_0^s F^{(5)}(t)\, dt\right] ds\right\}. \tag{12.2}$$

Evaluating the integral of the first term ds, interchanging the order of integration of the iterated integral, and computing the inner integral in the new iterated integral will all combine to give

$$\frac{-1}{h}\left\{\frac{-h^2}{2} F''(0) + \frac{h^4}{12} F^{(4)}(0) + \int_0^h \left[\frac{(h-t)^3}{12}(3t+h)\right] F^{(5)}(t)\, dt\right\}\ . \tag{12.3}$$

Here again one should note the sign of the "kernel" $\left[\frac{(h-t)^3}{12}(3t+h)\right]$; this time it is nonnegative on the interval of t between 0 and h, regardless of the sign of h.

The relation (12.3) can now be used in the calculations in (11.8) above, in place of the relation (11.7) that we previously used. It is useful in two special cases. In the special case where $h_i = h_{i-1} = h$ of (11.8) above, it is easy to check that not only do the two terms containing $f''(x_i)$ cancel, but also the two terms containing $f^{(4)}(x_i)$. As a result, the r. h. s. of the i-th equation for the $\{\epsilon_i\}$ takes the form

$$\frac{-1}{4h} \cdot \left\{\int_{-h}^0 \left[\frac{(h+t)^3}{12}(h-3t)\right] F^{(5)}(x_i - t)\, dt + \int_0^h \left[\frac{(h-t)^3}{12}(h+3t)\right] F^{(5)}(x_i + t)\, dt\right\}\ . \tag{12.4}$$

The integral of the "kernel" is $\frac{h^5}{30}$ on each of $[-h, 0]$ and $[0, h]$, so the entire expression (12.4) can be estimated in absolute value by $\frac{1}{4h} \cdot \frac{2h^5}{30} \cdot M_5 = \frac{h^4}{60} \cdot M_5$. This looks as though we have gained a whole "power-of-h" on our former error estimate (11.12)! That is too good to be true: all we have improved is our estimate of $\max\{|\epsilon_i| : 0 \le i \le n\} \le \frac{h^4}{60} M_5$, and although we get to multiply by $\frac{h}{4}$ in estimating $\max\{|e_i(x)| : x_0 \le x \le x_n\}$, we find that, as in (11.12), we still have to write

$$|f(x) - p_i(x)| \le |f(x) - H(x)| + |e_i(x)| \le \frac{h^4}{384} \cdot M_4 + \frac{h^5}{240} \cdot M_5\ ; \tag{12.5}$$

the first term is still of order h^4. Nonetheless, the second term still becomes small in comparison to the first, so for small values of $h > 0$ we can manage to get our error bounded by $\frac{h^4}{384} \cdot M_4 \cdot (1 + O(h))$—which is almost 5 times as optimistic as the best-generally-possible error estimate. But we shouldn't get our hopes up too high—even in the case of $f(x) = x^4$, whose 5-th derivative is identically zero and for which $e_i(x)$ vanishes identically on equally spaced nodes. The Hermite-interpolant part of the error will still produce the deviations shown in Fig. 2 $\{$where $f(x) = 1 - x^4$, $x_0 = -1$, $x_1 = 0$, and $x_2 = 1\}$ to remind us that the piecewise cubic will only resemble a curve that is not a cubic in case the pieces are fairly short. The "bulging" present even though the 1st and 2nd derivatives agree at the origin shows what to expect.

On the pessimistic side, we can see that for very disparate choices of h_i and h_{i+1} we have to expect considerable inaccuracy. Indeed, for 5-times-continuously differentiable $f(x)$ the expression (11.8) is now

$$\frac{-1}{2(h_{i-1} + h_i)} \left\{ \frac{h_i}{h_{i-1}} \cdot \frac{-h_{i-1}^4}{12} + \frac{h_{i-1}}{h_i} \cdot \frac{h_i^4}{12} \cdot f^{(4)}(x_i) + O(h^5) \right\} . \tag{12.6}$$

The absolute value of the coefficient of $f^{(4)}(x_i)$ in the leading term of this expression is

$$\left| \frac{1}{24} \frac{h_i h_{i-1} \cdot (h_i^2 - h_{i-1}^2)}{h_{i-1} + h_i} \right| = \frac{h_i h_{i-1} |h_i - h_{i-1}|}{24} . \tag{12.7}$$

To estimate this, do calculus: maximize $xy(y - x)$ on the triangle $0 \le x$, $0 \le y \le h$, $y \ge x$. The gradient of this function is $(y^2 - 2xy, 2xy - x^2)$ which has no zeros interior to the triangle, so the maximum is attained on the boundary—obviously not on the line $x = 0$ (!)—so therefore on the line $y = h$. Maximizing $hx(h - x)$ gives $x = h/2$, so the worst case of our estimate occurs for $h_i = h/2$, $h_{i-1} = h$ (or vice versa), and is $h^3/96$. It follows that at an x_i which divides the interval $[h_{i-1}, h_{i+1}]$ in the ratio 2:1, one must expect an ϵ_i of this size. Consequently, if the nodes $\{x_i : 0 \le i \le n\}$ divide the interval J in ratios alternately 1:2 and 2:1, one cannot expect a bound on the error cubics $e_i(x)$ which is much smaller than the numbers $\frac{h}{4} \cdot \frac{h^3}{96} \cdot |F^{(4)}(x_i)| = \frac{h^4}{384} \cdot |F^{(4)}(x_i)|$, and thus an error estimate on the order of

$$|f(x) - p_i(x)| \le \frac{2h^4}{384} \cdot M_4 \tag{12.8}$$

would be about the best one could really plan on. Fig. 3 shows what can happen $\{$with $f(x) = 1 - x^4$, $x_0 = -1$, $x_1 = -1/2$, $x_2 = 1/2$, $x_3 = 1\}$. The bulge is quite unexpectedly large, and worst at a point where $f(x)$ is very flat, so smoothness of the function $f(x)$ doesn't help at all.

13. Cubic spline interpolants of $f(x)$ have the further property that their derivatives manage to approximate the derivatives of $f(x)$, at least up to order 3. The work of proving this splits into two parts as before: estimate the error for the appropriate derivative of the Hermite interpolant on $[x_i, x_{i+1}]$, and then estimate the size of the appropriate derivative of $e_i(x)$.

For the first derivative of the Hermite interpolant on $[x_i, x_{i+1}]$, we have the exact error term

$$f[x_i, x_i, x_{i+1}, x_{i+1}, x](x - x_i)^2(x - x_{i+1})^2 \tag{13.1}$$

at x. Differentiating this with respect to x yields

$$\begin{aligned} &f[x_i, x_i, x_{i+1}, x_{i+1}, x, x](x - x_i)^2(x - x_{i+1})^2 + \\ &\quad f[x_i, x_i, x_{i+1}, x_{i+1}, x]\{2\,(x - x_i)(x - x_{i+1})^2 + 2\,(x - x_i)^2(x - x_{i+1})\} ; \end{aligned} \tag{13.2}$$

then plugging the identity

$$f[x_i, x_i, x_{i+1}, x_{i+1}, x, x] \cdot (x - x_i) = f[x_i, x_{i+1}, x_{i+1}, x, x] - f[x_i, x_i, x_{i+1}, x_{i+1}, x] \tag{13.3}$$

into the first term on the r. h. s. turns the differentiated error term into

$$f[x_i, x_{i+1}, x_{i+1}, x, x](x - x_i)(x - x_{i+1})^2 + f[x_i, x_i, x_{i+1}, x_{i+1}, x](x - x_i)(x - x_{i+1})^2 + 2(x - x_i)^2(x - x_{i+1}) . \tag{13.4}$$

Term-by-term estimation of the absolute value, with the 4-th-order divided differences estimated by $M_4/4!$, gives

$$\frac{M_4}{4!} \cdot (x_{i+1} - x)(x - x_i) \cdot [|x - x_{i+1}| + |(x - x_{i+1}) + 2(x - x_i)|] =$$
$$\frac{M_4}{4!} \cdot (x_{i+1} - x)(x - x_i) \cdot [x_{i+1} - x + |3x - (x_{i+1} + 2x_i)|] \ . \tag{13.5}$$

Because we are seeking a bound valid for all $f(x)$ and the geometry is symmetrical, we can restrict our attention to the case $x \le \dfrac{x_i + x_{i+1}}{2}$, *i.e.*, the case in which x lies in the left half of $[x_i, x_{i+1}]$. There are two cases according to whether $x \le \dfrac{2x_i + x_{i+1}}{3}$ or not, and it is routine calculus to verify that the largest value of the estimate occurs at the midpoint of $[x_i, x_{i+1}]$, giving the value

$$\frac{M_4}{4!} \cdot \frac{h_i^2}{4} \cdot \left[\frac{h_i}{2} + \frac{h_i}{2}\right] = \frac{M_4}{96} \cdot h^3 \ . \tag{13.6}$$

{Any interested reader seeking to verify this bound should move the origin of coordinates to the center of $[x_i, x_{i+1}]$ before doing the calculus.} This is not the sharpest-possible estimate, but the constants are adequate and the order of magnitude certainly correct.

For the first derivative of $e_i(x)$ on $[x_i, x_{i+1}]$, we have

$$\begin{aligned} h_i^2 \cdot \frac{d}{dx} e_i(x) &= \frac{d}{dx} \{(x - x_i)(x - x_{i+1})[\epsilon_{i+1}(x - x_i) + \epsilon_i(x - x_{i+1})]\} \\ &= (x - x_{i+1})[\epsilon_{i+1}(x - x_i) + \epsilon_i(x - x_{i+1})] + (x - x_i)[\epsilon_{i+1}(x - x_i) + \epsilon_i(x - x_{i+1})] \\ &\quad + (x - x_{i+1})(x - x_i)(\epsilon_{i+1} + \epsilon_i) \\ &= \epsilon_{i+1}(x - x_i)(x - 2x_{i+1} - x_i) + \epsilon_i(x - x_{i+1})(x - 2x_i - x_{i+1}) \ . \end{aligned} \tag{13.7}$$

This is majorized by

$$\max(|\epsilon_i|, |\epsilon_{i+1}|) \cdot [|(x - x_i)(x - 2x_{i+1} - x_i)| + |(x - x_{i+1})(x - 2x_i - x_{i+1})|] \tag{13.8}$$

and it is fairly easy, working case-by-case, to maximize the expression in square brackets in (13.8), obtaining just h_i^2. The derivative of $e_i(x)$ is thus bounded in absolute value by $\max\{|\epsilon_i|, |\epsilon_{i+1}|\}$. We can now estimate the error in approximating $f'(x)$ with $p_i'(x)$ by routine application of the triangle inequality:

$$\begin{aligned} |f'(x) - p_i'(x)| &\le |f'(x) - H'(x)| + |e_i'(x)| \\ &\le \frac{M_4}{96} \cdot h^3 + \max\{|\epsilon_i|, |\epsilon_{i+1}|\} \le \frac{M_4}{96} \cdot h^3 + \frac{M_4}{24} \cdot h^3 \quad \text{(use (11.10))} \\ &= \frac{M_4}{24} \cdot \frac{5}{4} \cdot h^3 \ . \end{aligned} \tag{13.9}$$

The best bound asserted in the literature is $\dfrac{M_4}{24} \cdot h^3$, so this one is adequate for our purposes.

Similar approaches will give estimates for f'' and $f^{(3)}$ of the form

$$|f''(x) - p_i''(x)| \le K_2 \cdot M_4 \cdot h^2 \qquad (K_2 \text{ some constant}) \tag{13.10}$$
$$|f^{(3)}(x) - p_i^{(3)}(x)| \le K_3 \cdot M_4 \cdot h \quad (K_3 \text{ some constant}); \tag{13.11}$$

one can apply the same method as above, viz., get a bound of the correct order for the error of the k-th derivative of the Hermite interpolant $H(x)$ on $[x_i, x_{i+1}]$ and get a bound of the correct order for the k-th derivative of $e_i(x)$ (the second and third derivatives of $e_i(x)$ will involve $1/h$ and $1/h^2$ respectively). The details are similar to those above, and are left as an exercise for any interested reader. I do not know what the best constants are, but K_3 is probably irrational.

It should perhaps be pointed out that since the $\{\epsilon_i\}$ are exactly the differences $\{b_i - f'_i\}$ between the derivative of the spline and the derivative of the function at the i-th node, the error $p'_i(x_i) - f'(x_i)$ in the approximation of the derivative *at the nodes* is on the order of h^4 when $f(x)$ is 5-times continuously differentiable and the nodes are equally spaced. {This follows from our investigation of that case above.} However, at points other than the nodes the order of approximation is the same as that of the derivative of the piecewise Hermite interpolant, which is only h^3. Still, this fact is occasionally useful in applications where a good approximate derivative at some point is desired: one just makes sure that that point is a node (and so perhaps one has to make one more measurement of an empirical $f(x)$).

14. Error in the Natural Spline Interpolant. This is the spline interpolant with zero curvature at the ends defined on p. 3 above. All we need do is look at the Taylor form of $p_i(x)$ at x_i (bottom of p. 7 above) and refer to Table 1 for the divided differences; we see that for $i = 0$ we have

$$\frac{1}{2!}\, p''_0(x_0) = \{f[x_0, x_1] - b_0\} - \left\{\frac{b_0 + b_1 - 2f[x_0, x_1]}{h_0}\right\} \tag{14.1}$$

so if we are to have $p''_0(x_0) = c_0$ (no harm in adding a little generality), that requirement replaces the 0-th equation in the system on p. 9 above by

$$2b_0 + b_1 = 3f[x_0, x_1] - c_0\,\frac{h_0}{2}\;. \tag{14.2}$$

Similarly, the n-th equation is replaced by

$$b_{n-1} + 2b_n = 3f[x_{n-1}, x_n] - c_n\,\frac{h_n}{2}\;. \tag{14.3}$$

The resulting matrix is just as strictly diagonally dominant as the one for the complete cubic spline, so it has the same solvability and "norm-reducing" properties that the previous one did. The natural cubic spline interpolant thus exists and is uniquely determined by $f(x)$ (as we already knew from the minimum-energy approach to splines).

There are some problems with the error estimates, however. We must now define ϵ_0 and ϵ_n by adjoining the equations

$$\begin{aligned} 2(f'_0 + \epsilon_0) + (f'_1 + \epsilon_1) &= 3f[x_0, x_1] - c_0\,\frac{h_0}{2} \quad \text{or} \\ 2\epsilon_0 + \epsilon_1 &= 3f[x_0, x_1] - f'(x_0) - 2f'(x_1) - c_0\,\frac{h_0}{2} \end{aligned} \tag{14.4}$$

and a similar equation at x_n, namely

$$\epsilon_{n-1} + 2\epsilon_n = 3f[x_{n-1}, x_n] - f(x_n) - 2f'(x_{n-1}) + c_n\,\frac{h_n}{2}\;. \tag{14.5}$$

The r. h. sides of these equations follow a familiar pattern, and it requires no more than imitation of the arguments above to see that they can be written in the form

$$\begin{aligned} 2\epsilon_0 + \epsilon_1 &= \frac{-1}{h_0}\left\{\frac{-h_0^2}{2} f''(x_0) + \frac{1}{2}\frac{h_0^4}{12} f^{(4)}(\xi_0)\right\} - c_0 h_0/2 \\ &= \frac{h_0}{2}\,[f''(x_0) - c_0] - \frac{h_0^3}{24}\, f^{(4)}(\xi_0) \end{aligned} \tag{14.6}$$

for some sample point $\xi_0 \in [x_0, x_1]$. A similar calculation at x_n gives

$$\epsilon_{n-1} + 2\epsilon_n = \frac{-h_n}{2}\,[f''(x_n) - c_n] + \frac{h_n^3}{24}\, f^{(4)}(\xi_n) \tag{14.7}$$

for some sample point $\xi_n \in [x_{n-1}, x_n]$. However, it is now evident that unless the forced second derivatives c_0 and c_n at the endpoints are chosen equal to the actual values of the second derivatives at the endpoints, we'll lose a factor of h^2 in our uniform estimate of the functions $|e_i(x)|$, $i = 0, \ldots, n$: the r. h. s. of the system of equations $AX = Y$ ($X =$ vector of ϵ_i's—$Y =$ r. h. sides of the equations above and the corresponding equations above) that we must solve is only bounded by a multiple of h instead of a multiple of h^3, and therefore we can expect a *uniform* error estimate that is only on the order of h^2 (recall the factor of $h/4$ that comes from the estimate in §10 above of $|e_i(x)|$ in terms of $\max\{|\epsilon_i| : i = 0, \ldots, n\}$).

The pessimistic appearance of this estimate is deceptive: the only reason that it looks so bad is that it is required to hold *uniformly* for all points $x \in [x_0, x_n]$. But it is *unreasonable* to expect good approximation near a endpoint at which one has wilfully forced a derivative of the spline to take a value that $f(x)$ thinks is wrong! Indeed, if c_0 and c_n are chosen equal to $f''(x_0)$ and $f''(x_n)$ in the estimate above, then the $O(h)$-terms drop out and the approximation becomes $O(h^4)$ as before. So in fact, the disturbance in the accuracy of the approximation turns out to be an *end effect*: the difference between a spline interpolant that does funny things at an endpoint and the complete cubic spline interpolant decays more rapidly than any power of h {or of 1/(the distance from x to the endpoint)} as $h \to 0$ or as x moves away from the endpoint, and so the order-of-magnitude estimates for the errors in other interpolants become indistinguishable from the ones we have developed for the complete cubic spline interpolant, once one gets away from the offending endpoint.

15. End Conditions other than the Complete End Conditions. The plan for investigating the approximation error of cubic spline interpolants with end conditions different from those of the complete spline parallels that used for the complete spline. We begin by setting up some notation.

Let $\{p_i(x) : 0 \le i < n\}$ and $\{b_i : 0 \le i \le n\}$ be the polynomials and slopes that define the complete cubic spline interpolant of the 4- or 5-times continuously differentiable function $f(x)$ on $[x_0, x_n]$. Let another cubic spline interpolant be defined by the cubic polynomials $\{q_i(x) : 0 \le i < n\}$ on the respective intervals $[x_i, x_{i+1}]$, with slopes $\{m_i : 0 \le i \le n\}$ at the nodes. Then their difference is a piecewise cubic function defined by $\{z_i(x) : 0 \le i < n\}$, with

$$q_i(x) = p_i(x) + z_i(x), \quad 0 \le i < n \ . \tag{15.1}$$

This piecewise cubic is twice-continuously-differentiable, since the two competing splines are, and it takes the value zero at all the nodes. Put

$$\zeta_i = m_i - b_i, \quad 0 \le i \le n \ . \tag{15.2}$$

Then, since both the $\{b_i : 1 \le i \le n-1\}$ and the $\{m_i : 1 \le i \le n-1\}$ satisfy the same equations

$$\begin{aligned} \mu_i b_{i-1} + 2b_i + \lambda_i b_{i+1} &= [\text{r. h. s. depending only on } f(x)] \\ \mu_i m_{i-1} + 2m_i + \lambda_i m_{i+1} &= [\text{r. h. s. depending only on } f(x)] \end{aligned}$$

at the interior nodes, their differences $\{\zeta_i : 1 \le i \le n-1\}$ satisfy the *homogeneous* equations

$$\mu_i \zeta_{i-1} + 2\zeta_i + \lambda_i \zeta_{i+1} = 0, \quad i = 1, ..., n-1 \ . \tag{15.3}$$

Suppose—in addition—that the $\{m_i : 0 \le i \le n\}$ satisfy two equations of the form

$$\begin{aligned} 2m_0 + \alpha_1 m_1 + \cdots + \alpha_n m_n &= k_0 \quad (\textstyle\sum |\alpha_i| \le 1,\ k_0 \text{ constant}) \\ \beta_0 m_0 + \beta_1 m_1 + \cdots + \beta_{n-1} m_{n-1} + 2m_n &= k_n \quad (\textstyle\sum |\beta_i| \le 1,\ k_n \text{ constant}). \end{aligned} \tag{15.4}$$

This format is certainly inclusive enough to include the case of the natural cubic spline interpolant in the preceding §. Then it is again clear that the matrix of coefficients is "strongly diagonally dominant" as in the discussion above, so the equations will have a unique solution. {Indeed, it would suffice to have $\sum |\alpha_i| < 2$ and $\sum |\beta_i| < 2$ to insure the solvability of the equations, and in fact all we need in what follows is that the equations be [uniquely] solvable for all choices of the numbers k_0 and k_n.}

In this case, however, we shall not control the $\{\zeta_i\}$ and the $|q_i(x)|$ by controlling the size of all the $\{\zeta_i\}$ *uniformly.* Rather, we shall control their size *away from the endpoints* by appealing to the equations

$$\mu_i\zeta_{i-1} + 2\zeta_i + \lambda_i\zeta_{i+1} = 0, \quad i = 1, ..., n-1\ . \tag{15.5}$$

For the sake of simplicity and because this is the most important case, consider the case where all $h_i = h$, so all $\mu_i = \lambda_i = 1/2$. Then the equations all have the form

$$1\zeta_{i-1} + 4\zeta_i + 1\zeta_{i+1} = 0, \quad i = 1, ..., n-1\ . \tag{15.6}$$

This is[9] a 2-*nd order linear homogeneous difference equation (with constant coefficients)* for the sequence $\{\zeta_i : 1 \le i \le n-1\}$. These are the discrete analogues of 2-nd order differential equations with constant coefficients. All such equations have solutions of the form

$$\zeta_i = (\text{const.}) \cdot r^i \tag{15.7}$$

where the number r can be determined by plugging the trial solution r^i into the difference equation, obtaining in the present case

$$(r^{i-1} + 4r^i + r^{i+1}) = r^{i-1} \cdot (r^2 + 4r + 1) = 0 \tag{15.8}$$

which is satisfied if and only if r satisfies the quadratic equation

$$(r^2 + 4r + 1) = 0 \Longleftrightarrow r = r_1 = -2 - \sqrt{3} \quad \text{or} \quad r = r_2 = -2 + \sqrt{3}\ . \tag{15.9}$$

(It is handy that $r_1 = r_2^{-1}$, and we shall use that fact without further reference). It is elementary to prove that *any* sequence $\{\zeta_i\}$ constructed from r_1 and r_2 by taking arbitrary constants A and B and setting

$$\zeta_i = A \cdot r_2^{-i} + B \cdot r_2^i \tag{15.10}$$

satisfies the difference equation, and that *every solution is of that form.* {For readers who want to check that assertion: determine A and B so that the values at $i = 1$ and $i = 2$ come out as the given sequence does, and by recursion all the values must come out the same.}

It is easy to check that the equations governing the ζ_i's are of the form

$$\begin{array}{cccccccccc}
2\zeta_0 & + & \alpha_1\zeta_1 & + & \cdots & + & \cdots & \alpha_n\zeta_n & = & K_0 \\
\vdots & & \vdots & \vdots & \vdots & & & \vdots & \vdots & \\
 & & \frac{1}{2}\zeta_{i-1} & + & 2\zeta_i & + & \frac{1}{2}\zeta_{i+1} & & = & 0 \\
\vdots & & \vdots & \vdots & \vdots & & & \vdots & \vdots & \\
\beta_0\zeta_0 & + & \beta_1\zeta_1 & + & \cdots & + & \beta_{n-1}\zeta_{n-1} & +2\zeta_n & = & K_n
\end{array} \tag{15.11}$$

where the numbers K_0 and K_n are two constants, different in general from the previous k_0 and k_n. Consider the system of equations with the same coefficient matrix

$$\begin{array}{cccccccc}
2\eta_0 & & & \cdots & & & = & 2C_0 \\
\vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 & \frac{1}{2}\eta_{i-1} & + & 2\eta_i & + & \frac{1}{2}\eta_{i+1} & = & 0 \\
\vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\
 & & & & & 2\eta_n & = & 2C_n
\end{array} \tag{15.12}$$

(9) For a thorough treatment of linear difference equations, please see the separate set of notes on this subject.

and solve these equations in the case where the r. h. s. is the "1-st standard basis vector" $(1,0,...,0)^T$ (so $C_0 = 1$, $C_n = 0$). For these equations we must have $\eta_n = 0$, $\eta_0 = 1$, and for $0 \le i \le n$ we must have

$$\eta_i = A \cdot r_2^{-i} + B \cdot r_2^i \tag{15.13}$$

for some constants A and B. Since these constants must satisfy

$$\begin{aligned} 1 &= \eta_0 = A + B \\ 0 &= \eta_n = A \cdot r_2^{-n} + B \cdot r_2^n \ , \end{aligned} \tag{15.14}$$

it is elementary to solve for the coefficients and find that

$$\eta_i = \frac{1}{1 - r_2^{2n}} \cdot [r_2^i - r_2^{2n-i}] \ . \tag{15.15}$$

The estimate

$$|\eta_i| \le \frac{1}{\sqrt{3}-1} \cdot 2 \cdot |r_2|^i = (\sqrt{3}+1) \cdot |r_2|^i \tag{15.16}$$

is just as elementary, since $2n - i \ge i$ holds for all $0 \le i \le n$ and $|r_2| < 1$. This estimate shows that the $|\eta_i|$ decay exponentially as i increases, and—of crucial importance—*the estimate of their size is independent of* n.

By symmetry or by repeating the argument, the solution of those equations with the r. h. s. $(0,0,...,0,1)^T$ is subject to a similar estimate

$$|\eta_i| \le (\sqrt{3}+1) \cdot |r_2|^{n-i} \ . \tag{15.17}$$

It follows {the reader should be sure to understand the details!} that the solutions of the equations as given are subject to the estimate

$$|\eta_i| \le (\sqrt{3}+1) \cdot \{|C_0| \cdot |r_2|^i + |C_n| \cdot |r_2|^{n-i}\} \ , \tag{15.18}$$

the r. h. s. of which is fairly small in the middle of the range of indices. Since the equations that originally determined the $\{\zeta_i\}$ can be rewritten in the form

$$\begin{array}{ccccccccc} 2\zeta_0 & & & & & & = & K_0 - \sum_i \alpha_i \zeta_i \\ \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\ & \frac{1}{2}\zeta_{i-1} & + & 2\zeta_i & + & \frac{1}{2}\zeta_{i+1} & = & 0 \\ \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\ & & & & & 2\zeta_n & = & K_n - \sum_i \beta_i \zeta_i \end{array} \tag{15.19}$$

we see that since it is known that $\max\{|\zeta_i|\} \le \max\{K_0, K_n\}$, the r. h. sides of the 0-th and n-th equations are bounded in absolute value by $2 \cdot \max\{K_0, K_n\}$, and so finally we see that the $|\zeta_i|$ are subject to the estimate

$$|\zeta_i| \le (\sqrt{3}+1) \cdot \max\{K_0, K_n\} \cdot [|r_2|^i + |r_2|^{n-i}] \ . \tag{15.20}$$

This setting is general enough to cover the case of the natural cubic spline interpolant: in this case the $i = 0$ equations are

$$\begin{aligned} 2b_0 &= 2f'(x_0) \quad \text{for the complete spline} \\ 2m_0 + m_1 &= 3f[x_0, x_1] \quad \text{for the natural spline} \end{aligned} \tag{15.21}$$

and thus

$$\begin{aligned}2(b_0+\zeta_0)+(b_1+\zeta_1) &= 3f[x_0,x_1]\\ 2\zeta_0+\zeta_1 &= 3f[x_0,x_1]-2f'(x_0)-b_1\\ &= 3f[x_0,x_1]-2f'(x_0)-f'(x_1)-\epsilon_1\end{aligned} \tag{15.22}$$

where ϵ_1 is the familiar "error in the derivative of the complete cubic spline interpolant at the node x_1". We know from the results of §13 above that the absolute value of the r .h. s. of this equation is actually of the form

$$-\frac{h}{2}\,f''(x_0)+O(h^3) \tag{15.23}$$

so it's certainly bounded. A similar equation and estimate are available for ϵ_n at the n-th node. Consequently the errors $\{\zeta_i : 0\le i\le n\}$ are subject to an estimate

$$|\zeta_i|\le K\cdot h\cdot[|r_2|^i+|r_2|^{n-i}] \tag{15.24}$$

where $K>0$ is some constant that we could estimate (in terms of M_2 and M_4, say) if it were important to do so.

The factor $[|r_2|^i+|r_2|^{n-i}]$ is "small in the middle of the range $1\le i\le n-1$" and we can exploit this to make the differences $\{z_i(x)\}$ between the splines small, in two ways. First, suppose we want error estimates that are valid uniformly in an interval $J(\delta)=[x_0+\delta,x_n-\delta]$, in which we "agree to stay at least a fixed distance $\delta>0$ from the endpoints." Then in order for the cell $[x_i,x_{i+1}]$ to be contained in $J(\delta)$—as a moment's geometrical thought will show—we must have $\delta/h\le i$ and $(\delta/h)+1\le n-i$. This gives

$$[|r_2|^i+|r_2|^{n-i}]\le(\text{const.})\cdot e^{-k\delta/h} \tag{15.25}$$

where $k=-\ln|r_2|\approx 1.3169579$; thus for $x\in J(\delta)$, we have an estimate

$$|\zeta_i|\le(\text{Const.})\cdot h\cdot e^{-k\delta/h} \tag{15.26}$$

whenever the index i belongs to an interval $[x_i,x_{i+1}]$ in which x can lie. As a result, using the estimate developed in §10 above for the cubic on $[x_i,x_{i+1}]$ with endpoint values 0, 0 and endpoint derivatives ϵ_i, ϵ_{i+1}, but replacing the ϵ's by ζ's, we see that we have an estimate

$$|z_i(x)|\le(\text{Const.})\cdot\frac{h^2}{4}\cdot e^{-k\delta/h} \tag{15.27}$$

valid uniformly for $x\in J(\delta)$. **Never mind the $\frac{h^2}{4}$—look at $e^{-k\delta/h}$, which $\to 0$ faster than any power of h as $h\to 0$!** {Use L'Hôpital's rule on $\ln(h^a e^{-k\delta/h})$ for $a\ge 0$—explicit bounds are also easy to compute.} Thus the difference between the natural cubic spline interpolant of $f(x)$ and its complete cubic spline interpolant "damps out like $e^{-1/h}$" uniformly in any fixed interval $J(\delta)$ contained in the open interval (x_0,x_n). The reader can easily see that this result can be applied to any of the cubic spline interpolants of more general type for which we set up the estimation machinery above.

Another way to look at the estimate we just derived is the following: take the estimate

$$|z_i(x)|\le(\text{Const.})\cdot\frac{h^2}{4}\cdot e^{-k\delta/h}\ , \tag{15.28}$$

let a small error tolerance $\eta>0$ be given, and try to make the r. h. s. of the estimate be $<h^4\eta$ by taking $\delta>2h$ sufficiently large. {Why h^4? because that is the order of the error in the complete cubic spline, and since we are estimating error as measured from that interpolant, there is no hope of improving the order of

the error estimate beyond that point. Why $2h$? Because we want to get into the "inside" of the interval J.}
Standard manipulation of

$$(\text{Const.}) \cdot \frac{h^2}{4} \cdot e^{-k\delta/h} < h^4 \eta \tag{15.29}$$

for $h < 1$ (so $\ln h = -|\ln h|$) leads to

$$\begin{aligned} -k\delta/h &< \ln(4\eta/(\text{Const.})) - 2|\ln h| \quad \text{or} \\ \delta &> \frac{1}{k} \cdot h \cdot [2|\ln h| - \ln(4\eta/(\text{Const.}))] \,. \end{aligned} \tag{15.30}$$

Because the expression in square brackets $\to \infty$ as $h \to 0$, we can make the r. h. s. of this inequality be $> 2h$ by taking h sufficiently small; and because $-\ln(4\eta/(\text{Const.}))$ is large and positive for small $\eta > 0$, once h is "sufficiently small" for such an it is also "sufficiently small" for all smaller η's. On the other hand, since $h|\ln h| \to 0$ as $h \to 0$, we can make the whole r. h. s. small by taking $h > 0$ sufficiently small. Thus there is a function of h—the r. h. s. of this inequality—which is of the order $O(h \ln h)$, such that for sufficiently small h, if $x \in [x_0, x_n]$ stays as far from x_0 and x_n as specified by that inequality, then the estimate

$$|f(x) - s(x)| \le \left[\frac{M_4}{384} + \eta\right] \cdot h^4 \tag{15.31}$$

holds, where $\eta > 0$ is any preassigned positive number. This result is valid for a large class of cubic spline interpolants including the natural one.(10)

Estimates of this type can be extended to the derivatives of cubic spline interpolants with little trouble by imitating the methods used for the natural spline above. The details can easily be filled in by the interested reader.

Attached figures with numbers > 3 show how the effects of the most wrong-headed choices of b_0 and b_n damp out quite quickly when the h_i are chosen equal and are only moderately small.

(10) This observation was made in the first ediction of Atkinson's book—cf. the inequality (3.84), p. 147—but was dropped from the second edition.