CUBIC SPLINES (an elementary approach)

The Weierstrass Approximation Theorem says that polynomials converge to $f \in C[a,b]$, but it does not say that interpolating polynomials converge. The Bernstein and Runge examples show that interpolating polynomials of higher and higher degree are not necessarily more accurate. Consider the error in polynomial interpolation:

$$f^{(n+1)}(\xi)\prod_{i=0}^{n}(x-x_i)/(n+1)!.$$

Since derivatives of f are usually an unknown quantity, the surest way to make the error small is to make the interval $[a,b]$ containing $x_0, \ldots, x_n$ small. Now the original interval $[a,b]$ is usually large, but one can interpolate on small subintervals, getting a *piecewise polynomial* approximation. The simplest case is a piecewise linear approximation, which is just a broken line.

Piecewise Hermite cubic. f is to be approximated by a piecewise cubic polynomial $g(x)$ with the properties that $g(x_i) = f(x_i)$, $g'(x_i) = f'(x_i)$, and $g(x)$ is a cubic polynomial $P_i(x)$ on each interval $[x_i, x_{i+1}]$, where $x_0 < x_1 < \cdots < x_n$. Newton's form for the Hermite cubic $P_i(x)$ in $[x_i, x_{i+1}]$ interpolates at x_i, x_i, x_{i+1}, x_{i+1} and is given by

$$P_i(x) = f[x_i] + f[x_i,x_i](x-x_i) + f[x_i,x_i,x_{i+1}](x-x_i)^2 + f[x_i,x_i,x_{i+1},x_{i+1}](x-x_i)^2(x-x_{i+1}).$$

Let $f_i = f(x_i)$, $s_i = f'(x_i)$, and rewrite $P_i(x)$ in terms of powers of $(x - x_i)$:

$$P_i(x) = c_{1,i} + c_{2,i}(x-x_i) + c_{3,i}(x-x_i)^2 + c_{4,i}(x-x_i)^3,$$

where

$$c_{1,i} = f_i, \qquad c_{2,i} = s_i, \qquad c_{3,i} = \frac{f[x_i,x_{i+1}] - s_i}{\Delta x_i} - c_{4,i}\Delta x_i, \qquad c_{4,i} = \frac{s_i + s_{i+1} - 2f[x_i,x_{i+1}]}{(\Delta x_i)^2}.$$

Note that $g(x)$ is C^1 on $[x_0, x_n]$, since $P_i'(x_{i+1}) = P_{i+1}'(x_{i+1}) = s_{i+1}$. $g(x)$ matches both f and f', so it is a good approximation to f, but it is not as "smooth" as it could be. By choosing the s_i, it is possible to construct a piecewise cubic which is C^2 and interpolates f. A C^2 curve is esthetically nicer than a C^1 curve; draftsmen can even "see" C^2 and C^3 discontinuities.

A C^2 piecewise cubic polynomial is called a *cubic spline*. In general,

Definition. A spline of degree m with nodes $x_0 < x_1 < \cdots < x_n$ is a C^{m-1} function which is a polynomial of degree $\le m$ in $(-\infty, x_0)$, (x_0, x_1), $\ldots$, (x_{n-1}, x_n), (x_n, ∞). A natural spline of degree $2k+1$ is a spline of degree $2k+1$ which is a polynomial of degree $\le k$ in $(-\infty, x_0)$ and (x_n, ∞).

The basic result is

Theorem. Let $0 \le k \le n$, $x_0 < x_1 < \cdots < x_n$. Then for any set of values $y_0, \ldots, y_n$ $\exists$ a unique natural spline $S(x)$ of degree $2k+1$ with nodes $x_0, \ldots, x_n$ such that $S(x_i) = y_i$ for $i = 0, 1, \ldots, n$.

Proof. Greville, *Theory and Applications of Spline Functions*, 1969.

Construction of a cubic spline (using first derivatives): In each interval $[x_i, x_{i+1}]$ the spline $g(x)$ has the form $P_i(x) = c_{1,i} + c_{2,i}(x - x_i) + c_{3,i}(x - x_i)^2 + c_{4,i}(x - x_i)^3$. The C^2 requirement means $P''_{i-1}(x_i) = P''_i(x_i) \Leftrightarrow 2c_{3,i-1} + 6c_{4,i-1}\Delta x_{i-1} = 2c_{3,i}$. Using the expressions for $c_{3,i}$, $c_{4,i}$ in terms of f_i, s_i (the s_i are now unspecified), this becomes

$$\Delta x_i s_{i-1} + 2(\Delta x_{i-1} + \Delta x_i)s_i + \Delta x_{i-1}s_{i+1} = 3\big(\Delta x_{i-1} f[x_i, x_{i+1}] + \Delta x_i f[x_{i-1}, x_i]\big), \ i = 1, \ldots, n-1.$$

These are $n-1$ linear equations in the $n+1$ unknowns s_0, ..., s_n. By specifying s_0, s_n, these become $n-1$ equations in $n-1$ unknowns, which have a unique solution since the coefficient matrix

$$\begin{pmatrix} 2(\Delta x_0 + \Delta x_1) & \Delta x_0 & 0 & 0 & \cdots \\ \Delta x_2 & 2(\Delta x_1 + \Delta x_2) & \Delta x_1 & 0 & \cdots \\ 0 & \Delta x_3 & 2(\Delta x_2 + \Delta x_3) & \Delta x_2 & \cdots \\ 0 & 0 & \Delta x_4 & 2(\Delta x_3 + \Delta x_4) & \ddots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix}$$

is strictly row diagonally dominant.

In summary, given $x_0 < x_1 < \cdots < x_n$ and $f(x_i)$, $i = 0, 1, \ldots, n$:

(1) Choose s_0, s_n (ideally $s_0 = f'(x_0)$, $s_n = f'(x_n)$, the *complete spline interpolant*).

(2) Solve the tridiagonal system of linear equations for s_1, ..., s_{n-1}.

(3) Construct the piecewise Hermite cubic $g(x)$ using $f(x_i)$ and s_i.

(4) Then $g(x)$ is a cubic spline on $[x_0, x_n]$ interpolating f at x_0, ..., x_n.

Construction of a cubic spline (using second derivatives): Let $g(x)$ be a piecewise cubic given by $P_i(x)$ on $[x_i, x_{i+1}]$, with $g''(x_i\pm) = s_i$, $i = 0, 1, \ldots, n$. Note that here the unknowns s_i are second derivatives. Since $P_i(x)$ is a cubic, $P''_i(x) = s_i(x_{i+1} - x)/\Delta x_i + s_{i+1}(x - x_i)/\Delta x_i$ is linear. Integrating twice and requiring that $P_i(x_i) = f(x_i) = f_i$, $P_i(x_{i+1}) = f(x_{i+1}) = f_{i+1}$ yields

$$\begin{aligned} P_i(x) = \frac{s_i}{6\Delta x_i}(x_{i+1} - x)^3 + \frac{s_{i+1}}{6\Delta x_i}(x - x_i)^3 + \left(\frac{f_{i+1}}{\Delta x_i} - \frac{s_{i+1}\Delta x_i}{6}\right)(x - x_i) \\ + \left(\frac{f_i}{\Delta x_i} - \frac{s_i \Delta x_i}{6}\right)(x_{i+1} - x), \qquad i = 0, 1, \ldots, n-1. \end{aligned}$$

So far the pieces $P_i(x)$ and their second derivatives match at the nodes. The first derivatives must also match, so another condition is $P'_{i-1}(x_i) = P'_i(x_i)$, $i = 1, \ldots, n-1$. This results in the following system of $n-1$ equations in the $n+1$ unknowns s_0, ..., s_n:

$$\Delta x_{i-1}s_{i-1} + 2(\Delta x_{i-1} + \Delta x_i)s_i + \Delta x_i s_{i+1} = 6\big(f[x_i, x_{i+1}] - f[x_{i-1}, x_i]\big), \qquad i = 1, \ldots, n-1.$$

Choosing s_0 and s_n uniquely determines the other s_i, since the coefficient matrix of the resulting linear system is strictly row diagonally dominant. The choice $s_0 = s_n = 0$ gives a *natural spline*.

In summary, given $x_0 < x_1 < \cdots < x_n$ and $f(x_i) = f_i$, $i = 0, 1, \ldots, n$:

(1) Choose $s_0 = s_n = 0$.

(2) Solve the tridiagonal linear system for s_i, $i = 1, \ldots, n-1$.

(3) Using these s_i, $g(x)$ given by $P_i(x)$ in $[x_i, x_{i+1}]$ is the unique natural cubic spline with nodes $x_0, x_1, \ldots, x_n$ interpolating f at $x_0, x_1, \ldots, x_n$.

Theorem. Let $f \in C^2[x_0, x_n]$, $x_0 < x_1 < \cdots < x_n$, $S(x)$ be the natural cubic spline interpolating f at $x_0, \ldots, x_n$, and let $g \in C^2[x_0, x_n]$ also interpolate f at $x_0, \ldots, x_n$. Then

$$\int_{x_0}^{x_n} \big(g''(x)\big)^2 dx \geq \int_{x_0}^{x_n} \big(S''(x)\big)^2 dx$$

with equality if and only if $g = S$.

Proof. $\int \big[g''(x) - S''(x)\big]^2 dx = \int \big(g''(x)\big)^2 dx - 2\int \big[g''(x) - S''(x)\big] S''(x) dx - \int \big(S''(x)\big)^2 dx$. The inequality will follow if the middle term is zero.

$$\begin{aligned}
\int_{x_0}^{x_n} (g'' - S'')S'' &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} (g'' - S'')S'' \\
&= \sum_{i=0}^{n-1} S''(x)\big(g'(x) - S'(x)\big)\Big|_{x_i}^{x_{i+1}} - \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} \big(g'(x) - S'(x)\big) S'''(x) dx \\
&= S''(x_n)\big(g'(x_n) - S'(x_n)\big) - S''(x_0)\big(g'(x_0) - S'(x_0)\big) \\
&\qquad - \sum_{i=0}^{n-1} \alpha_i \int_{x_i}^{x_{i+1}} \big(g'(x) - S'(x)\big) dx
\end{aligned}$$

since $S'''(x)$ is a constant α_i on (x_i, x_{i+1}).

$$\int_{x_i}^{x_{i+1}} \big(g'(x) - S'(x)\big) dx = g(x) - S(x)\Big|_{x_i}^{x_{i+1}} = 0$$

since both g and S interpolate f at $x_0, \ldots, x_n$. Also $S''(x_0) = S''(x_n) = 0$ since S is a natural cubic spline. Hence $\int \big(g'' - S''\big)^2 = \int (g'')^2 - \int (S'')^2 \geq 0 \Rightarrow \int (g'')^2 \geq \int (S'')^2$.

There is equality $\Leftrightarrow \int \big(g'' - S''\big)^2 = 0 \Leftrightarrow g'' - S'' = 0$ since g'' and S'' are continuous. Now $g'' = S'' \Rightarrow g(x) = S(x) + c_1 x + c_2$. But $g(x_0) = S(x_0)$, $g(x_1) = S(x_1)$, $x_1 \neq x_0 \Rightarrow c_1 x_0 + c_2 = 0$, $c_1 x_1 + c_2 = 0 \Rightarrow c_1 = c_2 = 0 \Rightarrow g(x) = S(x)$. Q. E. D.

Corollary. Let $f \in C^2[x_0, x_n]$, $x_0 < x_1 < \cdots < x_n$, $S(x)$ be the complete cubic spline interpolant to f at $x_0, \ldots, x_n$, with $S'(x_0) = f'(x_0)$, $S'(x_n) = f'(x_n)$, and let $g \in C^2[x_0, x_n]$ also interpolate f at $x_0, \ldots, x_n$, with $g'(x_0) = f'(x_0)$, $g'(x_n) = f'(x_n)$. Then

$$\int_{x_0}^{x_n} \big(g''(x)\big)^2 dx \geq \int_{x_0}^{x_n} \big(S''(x)\big)^2 dx$$

with equality if and only if $g = S$.

Theorem. Let $f \in C^2[a,b]$, $S(x)$ be the natural cubic spline interpolating f at $a = x_0 < x_1 < \cdots < x_n = b$, and $h = \max\limits_{0 \le i \le n-1}(x_{i+1} - x_i)$. Then

$$\|f - S\|_\infty \le h^{3/2} \|f''\|_2 \qquad \text{and} \qquad \|f' - S'\|_\infty \le h^{1/2} \|f''\|_2 .$$

Proof. Let $x \in [a,b]$. x is in some $[x_i, x_{i+1}]$, and since $f(t) - S(t)$ is zero at x_i and x_{i+1}, $f'(z) - S'(z) = 0$ for some $z \in (x_i, x_{i+1})$ by Rolle's Theorem. Then

$$\int_z^x \big[f''(t) - S''(t)\big]\, dt = f'(t) - S'(t)\Big|_z^x = f'(x) - S'(x).$$

Using the Cauchy-Schwarz Inequality,

$$\begin{aligned} |f'(x) - S'(x)| &= \left|\int_z^x \big[f''(t) - S''(t)\big] \cdot 1 dt\right| \le \left|\int_z^x \big[f''(t) - S''(t)\big]^2 dt\right|^{1/2} \left|\int_z^x 1^2 dt\right|^{1/2} \\ &\le \left|\int_z^x \big[f''(t) - S''(t)\big]^2 dt\right|^{1/2} h^{1/2}. \end{aligned}$$

From the previous theorem, with $g = f$, $\int_a^b \big[f''(t) - S''(t)\big]^2 dt = \int_a^b f''(t)^2 dt - \int_a^b S''(t)^2 dt \le \int_a^b f''(t)^2 dt$. Since z and x are in $[a,b]$,

$$|f'(x) - S'(x)| \le \left(\int_a^b f''(t)^2 dt\right)^{1/2} h^{1/2} = \|f''\|_2\, h^{1/2}.$$

Finally, $f(x) - S(x) = \int_{x_i}^x \big[f'(t) - S'(t)\big]\, dt$, so

$$\begin{aligned} |f(x) - S(x)| &= \left|\int_{x_i}^x \big[f'(t) - S'(t)\big]\, dt\right| \\ &\le \int_{x_i}^x \max_{[a,b]} |f'(\tau) - S'(\tau)| dt = \max_{[a,b]} |f'(\tau) - S'(\tau)| (x - x_i) \\ &\le \|f''\|_2\, h^{1/2} (x - x_i) \le \|f''\|_2\, h^{3/2}. \end{aligned}$$

Q. E. D.

Theorem (deBoor, 1978). Let $f \in C^4[a,b]$, $S(x)$ be the complete cubic spline interpolating f at $a = x_0 < x_1 < \cdots < x_n = b$, $S'(x_0) = f'(x_0)$, $S'(x_n) = f'(x_n)$, and $h = \max\limits_{0 \le i \le n-1}(x_{i+1} - x_i)$. Then

$$\left\|f^{(k)} - S^{(k)}\right\|_\infty = \mathcal{O}\big(h^{4-k}\big), \qquad k = 0, 1, 2.$$