properties that we shall now develop. First we note by a simple algebraic reduction that for any $g(x)$ and $S(x) \in C^2[a, b]$

$$\begin{aligned}\int_a^b [g''(x) - S''(x)]^2\,dx &= \int_a^b g''(x)^2\,dx - \int_a^b S''(x)^2\,dx \\ &\quad - 2\int_a^b S''(x)[g''(x) - S''(x)]\,dx.\end{aligned} \tag{5.48}$$

We concentrate on the last integral in (5.48) and see that integration by parts yields

$$\begin{aligned}&\int_a^b S''(x)[g''(x) - S''(x)]\,dx \\ &\qquad = S''(x)[g'(x) - S'(x)]\Big|_a^b - \int_a^b S'''(x)[g'(x) - S'(x)]\,dx.\end{aligned} \tag{5.49}$$

For the first extremal property we let $g(x)$ be any function in $C^2[a, b]$ that interpolates $f(x)$ at $\{x_j\}_{j=0}^n$. If $S(x) \in Sp(X_n)$, then $S'''(x)$ is a constant, say α_j, on each subinterval (x_j, x_{j+1}). Therefore

$$\begin{aligned}\int_a^b S'''(x)[g'(x) - S'(x)]\,dx &= \sum_{j=0}^{n-1} \alpha_j \int_{x_j}^{x_{j+1}} [g'(x) - S'(x)]\,dx \\ &= \sum_{j=0}^{n-1} \alpha_j [g(x) - S(x)]\Big|_{x_j}^{x_{j+1}} = 0\end{aligned}$$

since $g(x_j) = f(x_j) = S(x_j)$, $0 \le j \le n$.

Now if $S(x) = S^{(2)}(x)$ (the natural cubic spline), then $S''(b) = S''(a) = 0$; and so the integral on the left-hand side of (5.49) is zero. Using this result in (5.48) yields

$$\begin{aligned}\int_a^b g''(x)^2\,dx &= \int_a^b S''(x)^2\,dx + \int_a^b [g''(x) - S''(x)]^2\,dx \\ &\ge \int_a^b S''(x)^2\,dx.\end{aligned} \tag{5.50}$$

We leave it to the reader to show that equality holds in (5.50) if and only if $g(x) \equiv S^{(2)}(x)$. Hence, by (5.50), among all possible functions in $C^2[a, b]$ that interpolate $f(x)$ [including all of $Sp(X_n)$, all interpolating polynomials, and even $f(x)$ itself if $f''(x)$ is continuous], the integral $\int_a^b g''(x)^2\,dx$ is minimized if and only if $g(x) = S^{(2)}(x)$. This is the first extremal property and it explains the origin of the name "spline" for the mathematical approximation since the "strain energy" of the drafter's elastic rod is essentially proportional to the integral of the square of the second derivative, which we see is minimized by $S^{(2)}(x)$. The property is also called the "minimum curvature" property since the curvature of any approximation is essentially the integral of the square of the second derivative. Thus the oscillatory behavior of the approximation is minimized by $S^{(2)}(x)$. Yet another interpretation of (5.50) is that among all functions in $C^2[a, b]$ that interpolate $f(x)$, the natural cubic spline is closest to being a broken line since the broken line $q(x)$ has zero curvature; that is, $\int_a^b q''(x)^2\,dx = 0$. not quite

For the second extremal property we now restrict the function $g(x)$ in (5.49) to be in the smaller set of functions that interpolate $f(x)$ *and* also satisfy $g'(a) = f'(a)$ and $g'(b) = f'(b)$ (such as the Hermite interpolating polynomial, for instance). This time we let $\hat{S}(x) = S^{(1)}(x)$; so $\hat{S}'(a) = f'(a) = g'(a)$ and $\hat{S}'(b) = f'(b) = g'(b)$. Using this, we again see that the integral in (5.49) is zero. Therefore, by (5.48), for all $g(x)$ of this particular form.

$$\int_a^b g''(x)^2\,dx = \int_a^b \hat{S}''(x)^2\,dx + \int_a^b [g''(x) - \hat{S}''(x)]^2\,dx. \qquad (5.51)$$

[Equation (5.51) should not be confused with (5.50) since $g(x)$ is now more restricted, but note that $S^{(1)}(x)$ has minimum curvature in this smaller class of functions.] Now we let $u(x)$ be any cubic spline on the points $\{x_j\}_{j=0}^n$, whether it interpolates $f(x)$ or not. We then let $g(x) \equiv f(x) - u(x)$ and $S(x) \equiv S^{(1)}(x) - u(x)$. Note that $S(x)$ is still a cubic spline and has the properties that $S(x_j) = g(x_j)$, $0 \le j \le n$, and $S'(a) = g'(a)$ and $S'(b) = g'(b)$. Thus this particular choice of $g(x)$ and $S(x)$ can be used in (5.51) and yields $\int_a^b g''(x)^2\,dx \ge \int_a^b [g''(x) - S''(x)]^2\,dx$, or

$$\int_a^b \left[\frac{d^2f(x)}{dx^2} - \frac{d^2u(x)}{dx^2}\right]^2 dx \ge \int_a^b \left[\frac{d^2f(x)}{dx^2} - \frac{d^2S^{(1)}(x)}{dx^2}\right]^2 dx. \qquad (5.52)$$

[We leave it to the reader to verify that equality holds in (5.52) if and only if $u(x) = S^{(1)}(x) + \alpha x + \beta$.] Formula (5.52) is the second extremal property. It says that if we measure the distance between $f(x)$ and any cubic spline $u(x)$ by the formula $\int_a^b [f''(x) - u''(x)]^2\,dx$, then this distance is minimized when $u(x) = S^{(1)}(x)$ [so $S^{(1)}(x)$ is a "best approximation" to $f(x)$ in this sense]. In summary, among all cubic splines $u(x)$, the *error* $f(x) - u(x)$ has *minimum curvature* when $u(x) = S^{(1)}(x)$. Among all functions $g(x)$ in $C^2[a, b]$ that interpolate $f(x)$, the *function* with minimum curvature is $g(x) = S^{(2)}(x)$. Among all functions $g(x)$ that interpolate $f(x)$ and satisfy $g'(a) = f'(a)$, $g'(b) = f'(b)$, the function with minimum curvature is $g(x) = S^{(1)}(x)$.

We conclude this section by giving error bounds on the approximation of $f(x)$ by $S(x)$ *and* the approximation of $f'(x)$ by $S'(x)$ where $S(x)$ can be taken to be either $S^{(1)}(x)$ or $S^{(2)}(x)$. For the sake of notation we let the error function be given by $E(x) = f(x) - S(x)$ for $x \in [a, b]$. Then $E'(x) = f'(x) - S'(x)$ is the error of the derivative approximation. We also let

$$h \equiv \max_{0 \le j \le n-1} (x_{j+1} - x_j),$$

the maximum step size. Let x be any arbitrary fixed point in $[a, b]$; then there exists some j, $0 \le j \le n - 1$, such that $x \in [x_j, x_{j+1}]$. Since $E(x_j) = E(x_{j+1}) = 0$, by Rolle's theorem there exists a point $c \in [x_j, x_{j+1}]$ such that $E'(c) = 0$. Thus, $\int_c^x E''(t)\,dt = E'(x) - E'(c) = E'(x)$. By the Cauchy-Schwarz inequality (see Problem 9, Section 2.6, or Theorem 5.8, Section 5.3), we have

$$\begin{aligned} |E'(x)|^2 &= \left|\int_c^x E''(t) \cdot 1\,dt\right|^2 \le \left(\int_c^x E''(t)^2\,dt\right)\left(\int_c^x 1^2\,dt\right) \\ &\le \left(\int_c^x E''(t)^2\,dt\right)|x - c| \le h\int_c^x E''(t)^2\,dt. \end{aligned} \tag{5.53}$$

From either (5.50) or (5.51) we find

$$\begin{aligned} \int_c^x E''(t)^2\,dt &\le \int_a^b E''(t)^2\,dt = \int_a^b [f''(t) - S''(t)]^2\,dt \\ &= \int_a^b f''(t)^2\,dt - \int_a^b S''(t)^2\,dt \le \int_a^b f''(t)^2\,dt. \end{aligned}$$

Substituting this expression into (5.53) and taking square roots yield

$$|E'(x)| \equiv |f'(x) - S'(x)| \le h^{1/2}\left(\int_a^b f''(t)^2\,dt\right)^{1/2} \qquad \text{for all } x \in [a, b]. \tag{5.54}$$

Thus for $x \in [a, b]$, $|f'(x) - S'(x)|$ is bounded by an expression proportional to $h^{1/2}$.

Now, as above, let x be fixed in $[a, b]$ and thus $x \in [x_j, x_{j+1}]$ for some j. Since $\int_{x_j}^x E'(t)\,dt = E(x) - E(x_j) = E(x) - 0 = E(x)$, we have

$$|E(x)| = \left|\int_{x_j}^x E'(t)\,dt\right| \le \int_{x_j}^x \left(\max_{a \le z \le b} |E'(z)|\right) dt \le h \max_{a \le z \le b} |E'(z)|.$$

Then by (5.54) we have

$$|E(x)| \le h^{3/2}\left(\int_a^b f''(t)^2\,dt\right)^{1/2}, \tag{5.55}$$

giving a bound for $|f(x) - S(x)|$ that is proportional to $h^{3/2}$.

Formulas (5.54) and (5.55) are important as error bounds, but also since the bounds are independent of x, they tell us that if we increase the number of interpolating points in a manner such that $h \to 0$ as $n \to \infty$, then $S(x)$ and $S'(x)$ converge uniformly to $f(x)$ and $f'(x)$, respectively. The inequality (5.54) is also significant in that it tells us that $S'(\alpha)$ is a good approximation to $f'(\alpha)$ for $\alpha \in [a, b]$. Thus cubic splines can be used as a method to find a numerical approximation for not only $f(x)$ but $f'(x)$ as well (see Example 5.12). This property is not shared by interpolating polynomials, $p_n(x)$, as their oscillatory behavior tends to exaggerate the difference between $f'(x)$ and $p_n'(x)$, and one must be extremely cautious in using interpolating polynomials for the purpose of numerical differentiation.

With a more careful mathematical analysis, sharper error bounds can be derived. Typical results are the following from Hall (1968). If $f^{(iv)}(x)$ is continuous for $a \le x \le b$, then

$$|E(x)| \le (5/384)\|f^{(iv)}\|_\infty h^4 \qquad \text{and} \qquad |E'(x)| \le \left(\frac{9 + \sqrt{3}}{216}\right) \|f^{(iv)}\|_\infty h^3.$$

PROBLEMS, SECTION 5.2.6

1. To illustrate what can happen in even the simplest Hermite-Birkhoff interpolation problems, consider the following three problems.
   a) Find $p \in \mathcal{P}_3$ such that $p(0) = 1$, $p'(0) = 1$, $p'(1) = 2$, $p(2) = 1$.
   b) Find $p \in \mathcal{P}_3$ such that $p(-1) = 1$, $p'(-1) = 1$, $p'(1) = 2$, $p(2) = 1$.
   c) Find $p \in \mathcal{P}_3$ such that $p(-1) = 1$, $p'(-1) = -6$, $p'(1) = 2$, $p(2) = 1$.

   Using the method of undetermined coefficients, show that problem (a) has a unique solution, problem (b) has no solution, and problem (c) has infinitely many solutions.
2. Find the third-degree Hermite interpolating polynomial for $f(x) = \cos(x)$ on $[0.3, 0.6]$, and compare the results with those of Example 5.3 [$\sin(0.3) \approx 0.295520$ and $\sin(0.6) \approx 0.564642$].
3. Find in $\mathcal{P}_4$ the polynomial $p(x)$ that interpolates $f(x) = |x|$ as follows: $p(-2) = f(-2)$, $p'(-2) = f'(-2)$, $p(0) = f(0)$, $p(2) = f(2)$, and $p'(2) = f'(2)$. Compare your results with those of Example 5.12 to see that this polynomial is generally better than the interpolating polynomial but not as good as the cubic spline.
4. Write a set of subroutines that can be used to generate the natural cubic spline interpolator on equally spaced knots and that can be used to evaluate, differentiate, and integrate the resulting cubic spline. These subroutines could take the form outlined below.

   As a start, assume the main program has the first knot X0, the knot spacing H, and a value for N; the knots x_j are given by $x_j = \text{X0} + \text{J} * \text{H}$, $0 \le \text{J} \le \text{N}$. Also assume the main program has arrays DATA and YPP where $\text{DATA(J)} = f(x_j)$, and where