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Note

The Local Behavior of the Derivative of a Cubic Spline Interpolator

The derivative of a cubic spline interpolator is sometimes used to smooth a histogram [2]. An asymptotically precise estimate of the difference between the derivative of the cubic spline interpolator and the derivative of the function interpolated does not seem to be immediately available. Such an estimate is obtained in this note from known results, under the assumption of equal interval size, appropriate boundary data, and sufficient smoothness.

The Derivation

Let

$$f(x), \qquad 0 \leqslant x \leqslant 1, \tag{1}$$

be continuously differentiable up to fourth order.

Assume that

$$y_j = f(x_j), \qquad j = 0, 1, \ldots, n, \tag{2}$$

are given along with $f'(0), f'(1)$, where

$$x_j = jh, \qquad h = 1/n. \tag{3}$$

Let $S_n(x)$ be the cubic spline interpolator of f with knots at the points x_j such that $f'(0) = y_0' = S_n'(0), f'(1) = y_n' = S_n'(1)$. The numbers

$$M_j = S_n''(x_j), \qquad j = 0, 1, \ldots, n, \tag{4}$$

are called the moments of the spline function $S_n(x)$. Then

$$AM = d \tag{5}$$

with

$$A = \begin{bmatrix} 2 & \lambda_0 & & & \\ \mu_1 & 2 & \cdot & & 0 \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \lambda_{n-1} \\ & 0 & & \cdot & 2 \\ & & & & \mu_n \end{bmatrix}, \qquad M = \begin{bmatrix} M_0 \\ \vdots \\ M_n \end{bmatrix}, \qquad d = \begin{bmatrix} d_0 \\ \vdots \\ d_n \end{bmatrix}, \tag{6}$$

where $\lambda_0 = \mu_n = 1$, $\lambda_j = \mu_j = \frac{1}{2}$ if $j = 1,..., n-1$,

$$d_0 = \frac{6}{h}\left(\frac{y_1 - y_0}{h} - y_0'\right), \qquad d_n = \frac{6}{h}\left(y_n' - \frac{y_n - y_{n-1}}{h}\right)$$
$$d_j = \frac{3}{h}\left(\frac{y_{j+1} - 2y_j + y_{j-1}}{h}\right), \qquad j = 1,..., n-1, \tag{7}$$

(see [3]). Let

$$G = \begin{bmatrix} f''(x_0) \\ f''(x_1) \\ \vdots \\ f''(x_n) \end{bmatrix}, \qquad r = d - AG = A(M - G). \tag{8}$$

It has then been shown that

$$\begin{aligned} r_0 &= (h^2/4)[f^{(4)}(\tau_1) - 2f^{(4)}(\tau_2)] \quad \text{with} \quad \tau_1, \tau_2 \in [x_0, x_1] \\ r_j &= (h^2/8)[f^{(4)}(\tau_1) + f^{(4)}(\tau_2) - 2f^{(4)}(\tau_3) - 2f^{(4)}(\tau_4)] \\ &\qquad \text{with} \quad \tau_i \in [x_{j-1}, x_{j+1}], \quad j = 1,..., n-1, \\ r_n &= (h^2/4)[f^{(4)}(\tau_1) - 2f^{(4)}(\tau_2)] \quad \text{with} \quad \tau_1, \tau_2 \in [x_{n-1}, x_n], \end{aligned} \tag{9}$$

(see [3, p. 88]).

The derivative of the cubic spline $S_n(x)$ is given by

$$\begin{aligned} S_n'(x) = &- M_j \frac{(x_{j+1} - x)^2}{2h} + M_{j+1} \frac{(x - x_j)^2}{2h} \\ &+ \frac{y_{j+1} - y_j}{h} - \frac{h}{6}(M_{j+1} - M_j) \end{aligned} \tag{10}$$

if $x \in [x_j, x_{j+1}]$ (see [1]). The difference between $M_j = S_n''(x_j)$ and $f''(x_j)$ can be estimated, since A^{-1} can be written out explicitly and we shall make use of this. Let us first replace M_j by $f''(x_j)$ on the right of (10) to obtain

$$\begin{aligned} &-f''(x_j) \frac{(x_{j+1} - x)^2}{2h} + f''(x_{j+1}) \frac{(x - x_j)^2}{2h} \\ &+ \frac{y_{j+1} - y_j}{h} - \frac{h}{6}(f''(x_{j+1}) - f''(x_j)) \end{aligned} \tag{11}$$

and estimate this as well as we can. Now

$$\begin{aligned} y_{j+1} - y_j = f(x_{j+1}) - f(x_j) &= f(x) + f'(x)(x_{j+1} - x) + \frac{f''(x)}{2}(x_{j+1} - x)^2 \\ &+ \cdots \\ &- \left\{ f(x) + f'(x)(x_j - x) + \frac{f''(x)}{2}(x_j - x)^2 + \cdots \right\} \end{aligned} \tag{12}$$

$$= f'(x)\, h + \frac{f''(x)}{2}\,[(x_{j+1} - x)^2 - (x_j - x)^2]$$

$$+ \frac{f'''(x)}{3!}\,[(x_{j+1} - x)^3 - (x_j - x)^3]$$

$$+ \frac{f^{(4)}(x)}{4!}\,[(x_{j+1} - x)^4 - (x_j - x)^4] + \cdots.$$

Also,

$$\begin{aligned} &- f''(x_j)\frac{(x_{j+1} - x)^2}{2h} + f''(x_{j+1})\frac{(x - x_j)^2}{2h} \\ &= - \left[f''(x) + (x_j - x) f'''(x) + \frac{(x_j - x)^2}{2} f^{(4)}(x) + \cdots\right] \\ &\quad\times \frac{(x_{j+1} - x)^2}{2h} \\ &= + \left[f''(x) + (x_{j+1} - x) f'''(x) + \frac{(x_{j+1} - x)^2}{2} f^{(4)}(x) + \cdots\right] \\ &\quad\times \frac{(x_j - x)^2}{2h}, \end{aligned} \tag{13}$$

while

$$f''(x_{j+1}) - f''(x_j) = hf'''(x) + \tfrac{1}{2}[(x_{j+1} - x)^2 - (x_j - x)^2] f^{(4)}(x) + \cdots. \tag{14}$$

By making use of (12)–(14), we find that (11) is

$$\begin{aligned} f'(x) + \frac{f^{(4)}(x)}{4!}\left\{\frac{1}{h}\,[(x_{j+1} - x)^4 - (x_j - x)^4] - 2h[(x_{j+1} - x)^2 - (x_j - x)^2]\right\} \\ + o(h^3) \end{aligned} \tag{15}$$

if $x \in [x_j, x_{j+1}]$.

The additional contribution due to the error in replacing M_j by $f''(x_j)$ will now be estimated. The elements of A^{-1} are (see [1, p. 38])

$$\begin{aligned} A_{i,j}^{-1} &= \frac{\sigma^{j-i}(1 + \sigma^{2i})(1 + \sigma^{2n-2j})}{(2 + \sigma)(1 - \sigma^{2n})}, \qquad 0 < i \leqslant j < n \\ A_{i,n}^{-1} &= \frac{\sigma^{n-i}(1 + \sigma^{2i})}{(2 + \sigma)(1 - \sigma^{2n})}, \qquad 0 < i \leqslant n \\ A_{0,j}^{-1} &= \frac{2\sigma^{j}(1 + \sigma^{2n-2j})}{(2 + \sigma)(1 - \sigma^{2n})}, \qquad 0 < j < n \\ A_{0,n}^{-1} &= \frac{2\sigma^{n}}{(2 + \sigma)(1 - \sigma^{2n})}, \end{aligned} \tag{16}$$

with $\sigma = 3^{1/2} - 2$. Also, $A^{-1}_{i,j} = A^{-1}_{j,i}$, $0 < i, j < n$, while $A^{-1}_{i,j} = A^{-1}_{n-i,n-j}$ for all i, j.

Let us consider a fixed value x, $0 < x < 1$. Then for fixed $\epsilon > 0$ and $\epsilon < i/n, j/n < 1 - \epsilon$; $A^{-1}_{i,j}$ can just be approximated asymptotically by $\sigma^{|i-j|}/(2 + \sigma)$ and

$$\sum_i \frac{\sigma^{|j-i|}}{2 + \sigma} = \frac{(1 + \sigma)}{(1 - \sigma)(2 + \sigma)} = \frac{1}{3}. \tag{17}$$

The error in making the replacement of (10) by (11) can be seen to be

$$f^{(4)}(x)(h/24)[(x_{j+1} - x)^2 - (x_j - x)^2] + o(h^3) \tag{18}$$

if $x \in [x_j, x_{j+1}]$ by making use of (8). We give a detailed argument here. From (9), it follows that

$$(*) \qquad r_j = -2(h^2/8) f^{(4)}(x_j) + o(h^2), \qquad j = 1, \dots, n - 1.$$

Fix x, $0 < x < 1$, and let

$$x_j = [nx]/n,$$

where $[y]$ is the greatest integer less than or equal to y. Now

$$M_j - f''(x_j) = \sum_k A^{-1}_{j,k} r_k$$

$$= (a) + (b) = \sum_{|k-j| \geqslant m} + \sum_{|k-j| < m}$$

where m is taken to be a fixed but large positive integer. The expressions (a) and (b) are estimated separately. Notice that $j \simeq xn$, $n - j \simeq (1 - x)n$ as $n \to \infty$. From (16) it follows that

$$|A^{-1}_{j,k}| \leqslant 0.3^{|j-k|}$$

and so

$$|(a)| \leqslant \alpha(0.3)^m h^2,$$

where α is an absolute constant. Also, the points x_k are such that

$$|x_k - x| \leqslant (m + 1) h$$

for $|k - j| \leqslant m$ and so they approach x at the rate h. Using (*) and the continuous differentiability of f up to fourth order, it follows that

$$\left|(b) - \sum_{|k-j|\leqslant m} \frac{\sigma^{|j-k|}}{2+\sigma}\left(-2\,\frac{h^2}{8} f^{(4)}(x)\right)\right| = o(h^2).$$

Since m is arbitrary, we have

$$M_j - f''(x_j) = -\frac{1}{12} f^{(4)}(x)\, h^2 + o(h^2).$$

Likewise if j is replaced by $j+1$. The total error in replacing (10) by (11) is then given by (18). A theorem follows.

THEOREM. *Let f be a function defined on* [0, 1] *that is continuously differentiable up to fourth order. Consider any fixed point x, $0 < x < 1$. If $S_n(x)$ is the cubic spline which interpolates to $f(x)$ at the knots $x_j = jh$, $h = 1/n$ and which is such that $S_n'(0) = f'(0)$, $S_n'(1) = f'(1)$,* then

$$\begin{aligned} S_n'(x) - f'(x) &\\ = \frac{f^{(4)}(x)}{4!}&\left\{\frac{1}{h}\left[(x_{j+1} - x)^4 - (x_j - x)^4\right] - h\left[(x_{j+1} - x)^2 - (x_j - x)^2\right]\right\} \\ &+ o(h^3) \end{aligned} \tag{19}$$

if $x \in [x_j, x_{j+1}]$ as $n \to \infty$.

Even if the intervals between knots are not equal, as long as

$$\frac{\max(x_{j+1} - x_j)}{\min(x_{j+1} - x_j)} < \alpha < \infty,$$

one might expect a similar asymptotic result. We can deduce from the theorem a similar result for the error $S_n(x) - f'(x)$ in terms of $f^{(4)}(x)$.

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