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Endpoint Formulas for Interpolatory Cubic Splines*

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Abstract. In the absence of known endpoint derivatives, the usual procedure is to use a "natural" spline interpolant which Kershaw has shown to have $\mathcal{O}(h^4)$ error except near the endpoints. This note observes that either the use of appropriate finite-difference approximations for the endpoint derivatives or a proposed modification of the interpolation algorithm leads to $\mathcal{O}(h^4)$ error uniformly in the interval of approximation.

We consider the interpolation to a function $x \in C^4[a, b]$ by cubic splines. Let $\{a = t_0, t_1, \cdots, t_n = b\}$ be a set of knots and, throughout, let y denote a cubic spline interpolant to x so that $y(t_j) = x_j = x(t_j)$ for $j = 0, \cdots, N$. The construction of y may be given in terms of the values $\{x_j\}$ and $\{\kappa_j\}$ with $\kappa_j = y''(t_j)$ for $j = 0, \cdots, N$. Kershaw [1] provides the estimates

$$|x^{(k)}(t) - y^{(k)}(t)| \leqq c_k h^{2-k}\left[h^2 M + 8 \max_j\{|x''(t_j) - \kappa_j|\}\right], \tag{1}$$

for $a \leqq t \leqq b$ and $k = 0, 1, 2$; here, $h = \max_j\{t_{j+1} - t_j\}$ and $M = \sup\{|x^{(4)}(t)|: a \leqq t \leqq b\}$. For y to be a cubic spline, the values $\{\kappa_j\}$ must satisfy

$$\alpha_j\kappa_{j-1} + 2\kappa_j + (1 - \alpha_j)\kappa_{j+1} = 6d_j, \qquad j = 1, \cdots, N - 1, \tag{2}$$

where

$$h_j = t_{j+1} - t_j, \qquad \alpha_j = h_{j-1}/(h_{j-1} + h_j),$$

$$d_j = [(1 - \alpha_j)x_{j-1} - x_j + \alpha_j x_{j+1}]/h_{j-1}h_j.$$

Kershaw has shown [1] that the Eqs. (2), together with either

$$y'(a) = x'(a), \qquad y'(b) = x'(b) \tag{3.1}$$

(giving the $D - 1$ spline interpolant) or

$$\kappa_0 = x''(a), \qquad k_N = x''(b) \tag{3.2}$$

(giving the $D - 2$ spline interpolant), are sufficient to determine all the values $\{\kappa_0, \cdots, \kappa_N\}$, and hence y, in such a way that

$$\max_j\{|x''(t_j) - \kappa_j|\} = \mathcal{O}(h^2 M) \tag{4}$$

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which, with (1), gives the estimates

$$|x^{(k)}(t) - y^{(k)}(t)| \leqq \mathcal{O}(h^{4-k}M), \qquad k = 0, 1, 2, \tag{5}$$

uniformly on $[a, b]$.

The standard practice in the absence of information about $x'(a)$, $x'(b)$ or $x''(a)$, $x''(b)$ is to use the "natural spline" interpolant, using (2) together with

$$\kappa_0 = 0, \qquad \kappa_N = 0, \tag{3.3}$$

to determine the $\{\kappa_i\}$ and therefore y. In this case, it is shown in [1] that the estimate (5) still holds for t in the interior of the interval but that the error is of lower order, in general, for t within $\mathcal{O}(h \log h)$ of the endpoints. It is our present intention to provide two methods for retaining the estimate (5) uniformly on $[a, b]$ without *a priori* knowledge of endpoint derivatives.

Observe, first, that (3.1) is equivalent, in conjunction with the system (2) to the pair of equations

$$2\kappa_0 + \kappa_1 = 6d_0, \qquad \kappa_{N-1} + 2\kappa_N = 6d_N \tag{6}$$

with

$$\begin{aligned} d_0 &= [x_1 - x_0 - h_0 p]/h_0^2, \\ d_N &= -[x_N - x_{N-1} - h_{N-1} q]/h_{N-1}^2, \end{aligned} \tag{7}$$

where $p = x'(a)$ and $q = x'(b)$. The combined system (2) + (6) can be written in the form $\mathbf{A}\boldsymbol{\kappa} = \mathbf{d}$ with

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 0 & \cdots & & 0 \\ \alpha_1 & 2 & 1-\alpha_1 & 0 & & 0 \\ 0 & \alpha_2 & 2 & 1-\alpha_2 & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \\ 0 & \cdots & & 0 & 1 & 2 \end{bmatrix}, \quad \boldsymbol{\kappa} = \begin{bmatrix} \kappa_0 \\ \vdots \\ \kappa_N \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} d_0 \\ \vdots \\ d_N \end{bmatrix} \tag{8}$$

and we note that $||\frac{1}{2}\mathbf{A} - \mathbf{I}||_\infty = \frac{1}{2}$, so that

$$||\mathbf{A}^{-1}||_\infty = \tfrac{1}{2}||(\tfrac{1}{2}\mathbf{A})^{-1}|| \leqq \tfrac{1}{2}/[1 - ||\tfrac{1}{2}\mathbf{A} - \mathbf{I}||_\infty] = 1.$$

It follows that if we replace p by p_* and q by q_* in (7), leaving the vector $\mathbf{d}$ otherwise unchanged, no component of $\boldsymbol{\kappa}$ is altered by more than

$$6||\mathbf{A}^{-1}||_\infty \, ||d - d_*|| \leqq 6 \max\{|p - p_*|/h_0, |q - q_*|/h_{N-1}\}.$$

Thus, the estimate (4) continues to hold—and so (5) holds uniformly on $[a, b]$—if we take p_*, q_* to be approximations to p, q with accuracy $\mathcal{O}(h^3M)$. This can be done using appropriate four-point difference formulas; to be precise, we may define p_* by

$$p_* = a_0x_0 + a_1x_1 + a_2x_2 + a_3x_3,$$

where

$$
\begin{aligned}
a_1 &= (h_0 + h_1)(h_0 + h_1 + h_2)/h_0h_1(h_1 + h_2),\\
a_2 &= -(h_0 + h_1 + h_2)h_0/h_1h_2(h_0 + h_1),\\
a_3 &= (h_0 + h_1)h_0/(h_0 + h_1 + h_2)(h_1 + h_2)h_2,\\
a_0 &= -(a_1 + a_2 + a_3),
\end{aligned} \tag{9}
$$

and similarly for q_*.

One could, alternatively, use four-point difference formulas to obtain approximations to $x''(a)$, $x''(b)$ of accuracy $\mathcal{O}(h^2M)$ for use in (3.2). A simpler method, modifying the system (6) for $j = 1, N-1$ rather than directly approximating κ_0, κ_N, depends on the observation that

$$(1 - \alpha_j)x''(t_{j-1}) - x''(t_j) + \alpha_j x''(t_{j+1}) = \mathcal{O}(h^2M), \qquad j = 1, \cdots, N-1, \tag{10}$$

and, further, that

$$\alpha_j x''(t_{j-1}) + 2x''(t_j) + (1 - \alpha_j)x''(t_{j+1}) = 6d_j + \mathcal{O}(h^2M), \qquad j = 1, \cdots, N-1. \tag{11}$$

For $j = 1$, one may eliminate $x''(t_{j-1}) = x''(a)$ between (10) and (11) to obtain

$$(2 - \alpha_1)x''(t_1) + (1 - 2\alpha_1)x''(t_2) = 6(1 - \alpha_1)d_1 + \mathcal{O}(h^2M) \tag{12}$$

and, proceeding similarly for $j = N - 1$,

$$(2\alpha_{N-1} - 1)x''(t_{N-2}) + (1 + 2\alpha_{N-1})x''(t_{N-1}) = 6\alpha_{N-1}\, d_{N-1} + \mathcal{O}(h^2M). \tag{13}$$

We may divide (12) by $(1 - \alpha_1)$ and (13) by α_{N-1} and then combine these with (11), for $j = 2, \cdots, N-2$, to obtain the system $\mathbf{Bk} = 6\mathbf{d}' + \mathcal{O}(h^2M)$ where we have set

$$\mathbf{B} = \begin{bmatrix} 2+r & 1-r & 0 & \cdots & 0 \\ \alpha_2 & 2 & 1-\alpha_2 & & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \alpha_{N-2} & 2 & 1-\alpha_{N-2} \\ 0 & \cdots & 0 & 1-r' & 2+r' \end{bmatrix}, \quad \mathbf{k} = \begin{bmatrix} x''(t_1) \\ \vdots \\ x''(t_{N-1}) \end{bmatrix}, \quad \mathbf{d}' = \begin{bmatrix} d_1 \\ \vdots \\ d_{N-1} \end{bmatrix} \tag{14}$$

with $r = \alpha_1/(1 - \alpha_1)$, $r' = (1 - \alpha_{N-1})/\alpha_{N-1}$. Note that $\mathbf{B}$ is diagonally dominant and that imposing a bound on r, r' imposes a uniform bound (i.e., independent of N, h) on $||\mathbf{B}^{-1}||_\infty$. If we obtain $\boldsymbol{\kappa}$ by solving the system $\mathbf{B}\boldsymbol{\kappa}' = 6\mathbf{d}'$ $[\boldsymbol{\kappa}' = (\kappa_1, \cdots, \kappa_{N-1})^*]$ and subsequently setting

$$\kappa_0 = 6d_1 - \kappa_1 - \kappa_2, \qquad \kappa_n = 6d_{N-1} - \kappa_{N-1} - \kappa_{N-2} \tag{15}$$

then the boundedness of $||\mathbf{B}^{-1}||_\infty$ together with (10), (11) imply the estimate (4) and the estimates (5) follow uniformly on $[a, b]$ from (1).

Observe that if $h_0 = h_1$, then $\alpha_1 = \frac{1}{2}$ and (12) gives κ_1 by the usual three-point difference formula (accurate to $\mathcal{O}(h^2M)$ with this spacing); similarly for κ_{N-1} if $h_{N-2} = h_{N-1}$ so $\alpha_{N-1} = \frac{1}{2}$. In this case the original system (6) can be used for $j = 2, \cdots, N-2$ with $\kappa_1 = 2d_1$, $\kappa_{N-1} = 2d_{N-1}$ and, subsequently, $\kappa_0 = 2\kappa_1 - \kappa_2$ and

$\kappa_N = 2\kappa_{N-1} - \kappa_{N-2}$. Under normal circumstances, this last would seem to be the method of choice.

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