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 $O(h^4)$ 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 $O(h^4)$ 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

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

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

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

where

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

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

(3.1) \quad $y'(a) = x'(a), \quad y'(b) = x'(b)$

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

(3.2) \quad $\kappa_0 = x''(a), \quad \kappa_N = x''(b)$

(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

$$\max_j |x''(t_j) - \kappa_j| = O(h^4 M).$$

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which, with (1), gives the estimates
\begin{equation}
|x^{(k)}(t) - y^{(k)}(t)| \leq \Theta(h^{k-M}), \quad k = 0, 1, 2,
\end{equation}
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
\begin{equation}
\kappa_0 = 0, \quad \kappa_N = 0,
\end{equation}
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 \(\Theta(h \log h)\) 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
\begin{equation}
2\kappa_0 + \kappa_1 = 6d_0, \quad \kappa_{N-1} + 2\kappa_N = 6d_N
\end{equation}
with
\begin{equation}
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{equation}
where \(p = x'(a)\) and \(q = x'(b)\). The combined system (2) + (6) can be written in the form \(A\kappa = d\) with
\begin{equation}
A = \begin{bmatrix}
2 & 1 & 0 & \cdots & 0 \\
0 & \alpha_2 & 2 & 1 - \alpha_2 & \vdots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & 1 & 2
\end{bmatrix}, \quad \kappa = \begin{bmatrix}
\kappa_0 \\
\vdots \\
\kappa_N
\end{bmatrix}, \quad d = \begin{bmatrix}
d_0 \\
\vdots \\
d_N
\end{bmatrix}
\end{equation}
and we note that \(\|\frac{1}{2}A - I\|_\infty = \frac{1}{2}\), so that
\begin{equation}
\|A^{-1}\|_\infty = \frac{1}{\frac{1}{2}||\frac{1}{2}A^{-1}||} \leq \frac{1}{\frac{1}{2}}[1 - \|\frac{1}{2}A - I\|_\infty] = 1.
\end{equation}
It follows that if we replace \(p\) by \(p_*\) and \(q\) by \(q_*\) in (7), leaving the vector \(d\) otherwise unchanged, no component of \(\kappa\) is altered by more than \(6\|A^{-1}\|_\infty \|d - d_*\| \leq 6 \max \{|p - p_*|/h_0, |q - q_*|/h_{N-1}|\} \). 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 \(\Theta(h^3M)\). This can be done using appropriate four-point difference formulas; to be precise, we may define \(p_*\) by
\begin{equation}
p_* = a_0 x_0 + a_1 x_1 + a_2 x_2 + a_3 x_3,
\end{equation}
where
\[
\begin{align*}
    a_1 &= (h_0 + h_1)(h_0 + h_1 + h_2)/h_0 h_1 (h_1 + h_2), \\
    a_2 &= -(h_0 + h_1 + h_2)h_0/h_1 h_2 (h_0 + h_1), \\
    a_3 &= (h_0 + h_1)h_0/(h_0 + h_1 + h_2) (h_1 + h_2) h_2, \\
    a_0 &= -(a_1 + a_2 + a_3),
\end{align*}
\]

and similarly for \( q_n \).

One could, alternatively, use four-point difference formulas to obtain approximations to \( x'(a) \), \( x''(b) \) of accuracy \( \Theta(h^2 M) \) for use in (3.2). A simpler method, modifying the system (6) for \( j = 1, N - 1 \) rather than directly approximating \( \kappa_0, \kappa_N \), depends on the observation that

\[
(10) \quad (1 - \alpha_j)x''(t_{j-1}) - x''(t_j) + \alpha_j x''(t_{j+1}) = 0(A^2 M), \quad j = 1, \cdots, N - 1,
\]

and, further, that

\[
(11) \quad \alpha_i x''(t_{i-1}) + 2x''(t_i) + (1 - \alpha_i)x''(t_{i+1}) = 6d_i + \Theta(h^2 M), \quad j = 1, \cdots, N - 1.
\]

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

\[
(12) \quad (2 - \alpha_1)x''(t_1) + (1 - 2\alpha_1)x''(t_2) = 6(1 - \alpha_1)d_1 + \Theta(h^2 M)
\]

and, proceeding similarly for \( j = N - 1 \),

\[
(13) \quad (2\alpha_{N-1} - 1)x''(t_{N-2}) + (1 + 2\alpha_{N-1})x''(t_{N-1}) = 6\alpha_{N-1} d_{N-1} + \Theta(h^2 M).
\]

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

\[
\begin{align*}
    B & = \begin{bmatrix}
        2 + r & 1 - r & 0 & \cdots & 0 \\
        \alpha_2 & 2 & 1 - \alpha_2 & 0 & \cdots \\
        0 & \cdots & \cdots & \cdots \\
        \cdots & \cdots & \alpha_{N-2} & 2 & 1 - \alpha_{N-2} \\
        0 & \cdots & 0 & 1 - r' & 2 + r'
    \end{bmatrix}, \quad k = \begin{bmatrix}
        x''(t_1) \\
        \vdots \\
        \vdots \\
        x''(t_{N-1})
    \end{bmatrix}, \quad d' = \begin{bmatrix}
        d_1 \\
        \vdots \\
        \vdots \\
        d_{N-1}
    \end{bmatrix},
\end{align*}
\]

with \( r = \alpha_1/(1 - \alpha_1), \ r' = (1 - \alpha_{N-1})/\alpha_{N-1} \). Note that \( B \) is diagonally dominant and that imposing a bound on \( r, r' \) imposes a uniform bound (i.e., independent of \( N, h \)) on \( \|B^{-1}\|_\infty \). If we obtain \( k \) by solving the system \( Bk' = 6d' \) \( k' = (k_1, \cdots, k_{N-1})^* \) and subsequently setting

\[
(15) \quad \kappa_0 = 6d_1 - k_1 - k_2, \quad \kappa_n = 6d_{N-1} - k_{N-1} - k_{N-2}
\]

then the boundedness of \( \|B^{-1}\|_\infty \) 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 \( k_1 \) by the usual three-point difference formula (accurate to \( \Theta(h^2 M) \) with this spacing); similarly for \( \kappa_{N-1} \) 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 \( k_1 = 2d_1, \kappa_{N-1} = 2d_{N-1} \) and, subsequently, \( \kappa_0 = 2k_1 - k_2 \) 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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