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Boundary Expansions for Spline Interpolation

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Abstract. An explicit method is given for deriving the formulae for derivatives of the spline of order $m + 1$ at two boundaries $x = a$, $x = b$ in terms of known function values and computed mth derivatives of the spline.

1. Introduction. General formulae for computing the spline $s(x)$ of degree $m + 1$ on a partition $a = x_0 < x_1 < \cdots < x_n = b$ of the interval $[a, b]$ have been considered with various types of boundary conditions in several previous papers (Ahlberg, Nilson and Walsh [1], Späth [5]).

However, the spline interpolation problem may always be formulated as the solution of a matrix equation where the matrix of coefficients is of band type with width $m + 1$. The special case of periodic boundary conditions yields a predominantly band matrix which is of circulant form (Hoskins and King [3]).

In the case when $s^{(q)}(x_j)$ $(j = 0, n;\ q = 1, 2, \cdots, m - 1)$ or, more generally, when linear combinations of these quantities are given, or, alternatively, when they merely require to be determined from the computed set of mth derivatives, it is not apparent from the development by Ahlberg et al. [1, pp. 124–132] that they may be obtained explicitly for all forms of boundary conditions solely in terms of values of the function and mth derivatives. Further, the explicit form for these conditions is such that the band structure of the matrix of coefficients may be retained.

2. Development of the Expansions. The polynomial spline $s(x)$ of degree $m + 1$ has as its $(m + 1)$st derivative

$$s^{(m+1)}(x) = \frac{s_j^{(m)} - s_{j-1}^{(m)}}{h_j}, \qquad j = 1, 2, \cdots, n, \tag{2.1}$$

where $x_{j-1} \leqq x \leqq x_j$, $h_j = x_j - x_{j-1}$ and $s_j^{(m)}$ denotes the mth derivative of $s(x)$ evaluated at $x = x_j$. Now the function $s(x)$ can be represented over the complete range $[x_0, x_n]$ in the form

$$s(x) = \sum_{k=0}^{m} \frac{x^k}{k!} s_0^{(k)} + \sum_{t=0}^{n-1} \frac{d_t}{(m + 1)!} (x - x_t)_+^{m+1} \tag{2.2}$$

where

$$\begin{aligned} z_+ &= z, & z &\geqq 0, \\ &= 0, & z &< 0 \end{aligned}$$

(Powell [4]). Using Eqs. (2.1) and (2.2) it is seen that

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$$
\begin{aligned}
d_0 &= (s_1^{(m)} - s_0^{(m)})/h_1, \quad \text{and} \\
d_t &= (s_{t+1}^{(m)} - s_t^{(m)})/h_{t+1} - (s_t^{(m)} - s_{t-1}^{(m)})/h_t, \qquad 0 < t < n-1,
\end{aligned} \tag{2.3}
$$

and, if Eq. (2.2) is expanded about the values x_k ($k = 1, 2, \cdots, m-1$), then

$$
s_k = \sum_{i=0}^{m} \frac{x_k^i}{i!} s_0^{(i)} + \sum_{i=0}^{k-1} \frac{d_i}{(m+1)!} (x_k - x_i)^{m+1}
$$

with slight rearrangement producing

$$
\sum_{i=1}^{m-1} \frac{x_k^i}{i!} s_0^{(i)} = s_k - s_0 - \sum_{i=0}^{k-1} \frac{(x_k - x_i)^{m+1}}{(m+1)!} \cdot d_i - \frac{x_k^m}{m!} s_0^{(m)}, \tag{2.4}
$$

$$
k = 1, 2, \cdots, m-1.
$$

The complete set of Eqs. (2.4) may be written in matrix form as

$$
A\mathbf{v} = \mathbf{b} \tag{2.5}
$$

where $A = \{x_i^j\}$ and is $(m-1) \times (m-1)$, $\mathbf{v} = \{s_0', s_0''/2!, \cdots, s_0^{(m-1)}/(m-1)!\}^T$ and the vector $\mathbf{b}$ has elements

$$
b_k = s_k - s_0 - \sum_{i=0}^{k-1} \frac{(x_k - x_i)^{m+1}}{(m+1)!} \cdot d_i - \frac{x_k^m}{m!} s_0^{(m)}, \qquad k = 1, 2, 3, \cdots, m-1.
$$

The quantities d_i appearing on the right-hand side of Eq. (2.5) are of course already given from Eqs. (2.3) in terms of mth derivatives, hence $\mathbf{v}$ defined as the solution of (2.5) gives the required expansions for $s_0^{(q)}$ ($q = 1, 2, \cdots, m-1$).

The coefficient matrix A is a special form of the Vandermonde matrix and possesses a well-known inverse (Gregory and Karney [2]) so that explicit expansions for the elements of $\mathbf{v}$ could be obtained if desired. However, from the computing aspect it is more economical to work directly with the system of Eqs. (2.5) when numerical values for the elements of $\mathbf{v}$ are required. In particular, if the partition of $[x_0, x_n]$ is uniform and $x_i = x_0 + ih$ where $h = (x_n - x_0)/n$ and $i = 0, 1, 2, \cdots, n$, then Eq. (2.5) can be simplified by associating the appropriate powers of h with the derivatives appearing in $\mathbf{v}$, and the matrix A becomes $A = \{i^j\}$. In this case, the vector $\mathbf{v}$ is easily obtained by solving the equivalent set of equations

$$
U\mathbf{v} = L\mathbf{b} \tag{2.6}
$$

where $U = \{\Delta^i 0^j\}$ and $L = \{(-1)^{i+j}\binom{i}{j}\}$, with $\Delta^i 0^j$ representing the ith difference of $i^j|_{i=0}$. Equation (2.6) is such that U is an upper triangular matrix and thus the determination of $\mathbf{v}$ is easily effected.

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