De Boor–Fix functionals and Hermite boundary conditions in the polynomial spline interpolation problem

Yuriy S. Volkov[1,2]

Abstract

By means of de Boor–Fix functionals Hermite boundary conditions in the problem of spline interpolation are obtained. It is shown that some of the first and last B-spline coefficients can be found by explicit formulas in terms of elementary symmetric functions and the remaining coefficients can be computed as a solution of a banded system of linear equations.

Keywords De Boor–Fix functionals · Spline interpolation · Hermite boundary conditions · Banded system of equations

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1 Definitions

Consider the space of splines of degree m (or order $m + 1$) on the interval $[a, b]$ with the sequence of knots

$$\delta: \ a = \xi_0 \leqslant \xi_1 \leqslant \cdots \leqslant \xi_k = b$$

where $\xi_i < \xi_{i+m+1}$. As a basis, we choose B-splines $N_i = N_{i, m+1, \delta}$ of degree m, i.e., N_i is given by the rule

$$N_i(x) = N_{i, m+1, \delta}(x) = \big([\xi_{i+1}, \ldots, \xi_{i+m+1}] - [\xi_i, \ldots, \xi_{i+m}]\big)(\cdot - x)^m_+, \quad (1)$$

✉ Yuriy S. Volkov
  volkov@math.nsc.ru

1 Sobolev Institute of Mathematics, 4 Koptuga Av., Novosibirsk, Russia 630090

2 Novosibirsk State University, 2 Pirogova St., Novosibirsk, Russia 630090

with $[\xi_j, \ldots, \xi_{j+r}]g$ the r-th divided difference of g at the points $\xi_j, \ldots, \xi_{j+r}$. In particular,

$$N_i(x) > 0 \quad \text{on} \ (\xi_i, \xi_{i+m+1})$$

and

$$N_i(x) = 0 \quad \text{off} \ (\xi_i, \xi_{i+m+1});$$

to be more exact $N_i(\xi_i) = 1$ in the case $\xi_i = \xi_{i+m}$ since splines are usually taken to be continuous from the right. To define the basis uniquely, it is necessary to specify an extension of the mesh to the left and right by m knots

$$\xi_{-m} \leqslant \xi_{-m+1} \leqslant \cdots \leqslant \xi_0, \qquad \xi_k \leqslant \xi_{k+1} \leqslant \cdots \leqslant \xi_{k+m}. \tag{2}$$

Then the sequence of B-splines N_i, $i = -m, \ldots, k - 1$, will be a basis of the space of splines of degree m on the extended mesh δ of $[a, b]$. Hence any spline s of degree m on the mesh δ can be uniquely represented in this basis as

$$s(x) = \sum_{i=-m}^{k-1} \alpha_i N_i(x) \tag{3}$$

with some coefficients $\alpha_{-m}, \ldots, \alpha_{k-1}$.

2 De Boor–Fix functionals

De Boor and Fix in the paper [2] introduced functionals λ_i^m defined by the formula

$$\lambda_i^m g := \sum_{r=0}^{m} (-1)^{m-r} \psi_{i,m}^{(m-r)}(\tau_i) g^{(r)}(\tau_i) \tag{4}$$

with $\tau_i \in (\xi_i, \xi_{i+m+1})$,

$$\psi_{i,m}(x) := \frac{1}{m!} (\xi_{i+1} - x) \cdots (\xi_{i+m} - x). \tag{5}$$

These functionals are interesting to us because when they act on an arbitrary spline of degree m on the mesh δ, we obtain the value of the coefficient α_i for N_i in the B-spline representation, i.e.,

$$\lambda_i^m s = \lambda_i^m \left(\sum_{j=-m}^{k-1} \alpha_j N_j \right) = \alpha_i.$$

In other words, any coefficient α_i in the B-spline representation can be expressed in terms of the values of this spline and its derivatives at some point $\tau_i \in (\xi_i, \xi_{i+m+1})$:

$$\alpha_i = \sum_{r=0}^{m} (-1)^{m-r} \psi_{i,m}^{(m-r)}(\tau_i) s^{(r)}(\tau_i). \tag{6}$$

It is clear that if the point τ_i is a mesh knot ξ_j for some j with $i \leqslant j \leqslant i + m + 1$, then in the sum (6) there will be derivatives only up to order $m - 1$.

More generally, if τ_i appears s-fold in the sequence $\xi_{i+1}, \ldots, \xi_{i+m}$, then $\psi_{i,m}$ has a zero of order s at τ_i, hence only the terms with $m - r \geqslant s$ in (6) are not obviously zero. Put differently, in this case, α_i is expressed as a weighted sum of $s^{(r)}(\tau_i), r = 0, \ldots, m - s$. And if

$$\tau_i = \xi_{i+1} = \cdots = \xi_{i+m},$$

then $\alpha_i = s(\tau_i)$, since, in this case $\psi_{i,m}$ has a zero of order m at τ_i, hence only the $r = 0$ term in (6) is not obviously zero.

This observation proves useful in the *complete* spline interpolation problem which is characterized by the fact that the endpoint conditions are Hermite conditions.

3 Complete spline interpolation

Consider the interpolation problem by polynomial splines on the segment $[a, b]$. In order to solve the problem uniquely, in addition to known values at the nodes of some mesh (if there is less than $k + m$ of them) more conditions are needed. The boundary conditions in the form of a certain number of derivatives at the endpoints of the segment (Hermitian boundary conditions) are most commonly used, which we will consider. For the classical splines of odd degree $m = 2n + 1$, n lower derivatives of the interpolated function are given at each endpoint of the interval [1]. When the spline degree is even $m = 2n$, in Subbotin's scheme [4,5] these are the same boundary conditions, but the spline knots are located strictly in the middle between the interpolation points. (There is also Marsden's scheme of interpolation by even degree splines [3], in which, on the contrary, the interpolation points are selected in the middle between the spline knots, see also [8,9].)

Let the interpolated values $f_0, \ldots, f_l$ be given on the mesh

$$\Delta: \quad a = x_0 < x_1 < \cdots < x_l = b$$

and $f_a^{(r)}, f_b^{(r)}, r = 1, \ldots, n$, be the values of derivatives up to order n at endpoints a and b. For splines of odd degree the meshes δ (knot mesh) and Δ (data mesh) coincide and $k = l$. But for splines of even degree in Subbotin's scheme

$$\xi_i = \frac{x_{i-1} + x_i}{2},$$

$i = 1, \ldots, l$, and $l = k - 1$. Further, it is convenient to consider additional nodes of the mesh Δ as multiple:

$$\cdots = x_{-1} = x_0, \qquad x_l = x_{l+1} = \cdots$$

and then additional knots (2) will be multiple too, i.e.,

$$\xi_{-m} = \xi_{-m+1} = \cdots = \xi_0, \qquad \xi_k = \xi_{k+1} = \cdots = \xi_{k+m}.$$

If coefficients of the spline expansion in the basis of the B-splines (3) are chosen as the defining parameters of the required interpolation spline, then the problem consists of finding the coefficients $\alpha_{-m}, \ldots, \alpha_{k-1}$. The system of linear equations for these parameters is immediately obtained from interpolation conditions

$$\sum_{j=-m}^{k-1} \alpha_j N_j(x_i) = f_i, \qquad i = 0, \ldots, l, \tag{7}$$

for given values $\{f_i\}$ and from boundary conditions

$$\sum_{j=-m}^{k-1} \alpha_j N_j^{(r)}(x_0) = f_a^{(r)}, \quad \sum_{j=-m}^{k-1} \alpha_j N_j^{(r)}(x_l) = f_b^{(r)}, \qquad r = 1, \ldots, n, \tag{8}$$

for the given values of derivatives $f_a^{(r)}$, $f_b^{(r)}$. In both cases for splines of odd and even degree, the relations (7) lead to a $(2n + 1)$-banded system of equations, but the expressions (8) break the band structure.

4 The banded system of equations

Instead of the relations (8) we propose to use the representation of the first and last $n+1$ coefficients $\{\alpha_j\}$ from the de Boor–Fix functionals and our observation for multiple knots. We obtain explicit formulas for these coefficients which we will express in terms of elementary symmetric functions of several variables

$$\mathrm{sym}_r^m(t_1, \ldots, t_m) := \sum_{1 \leqslant i_1 < i_2 < \cdots < i_r \leqslant m} t_{i_1} \cdots t_{i_r}$$

or

$$\mathrm{sym}_0^m(t_1, \ldots, t_m) = 1,$$
$$\mathrm{sym}_1^m(t_1, \ldots, t_m) = t_1 + \cdots + t_m,$$
$$\mathrm{sym}_2^m(t_1, \ldots, t_m) = t_1 t_2 + t_1 t_3 + \cdots + t_{m-1} t_m,$$
$$\cdots$$
$$\mathrm{sym}_m^m(t_1, \ldots, t_m) = t_1 \cdots t_m.$$

Theorem 4.1 *If the polynomial spline s of some degree m with knots in the mesh δ interpolates the given values* $\{f_i\}$ *on the mesh* Δ *and* $\alpha_{-m}, \ldots, \alpha_{k-1}$ *are the coefficients of the spline expansion in the basis of the B-splines for s then the first and last* $n + 1$ *coefficients can be found by the following explicit formulas:*

$$\alpha_{-m+i} = \sum_{r=0}^{i} \frac{(m-r)!}{m!} \operatorname{sym}_r^i(\xi_1 - \xi_0, \ldots, \xi_i - \xi_0) f_a^{(r)}, \tag{9}$$

$$\alpha_{k-1-i} = \sum_{r=0}^{i} \frac{(m-r)!}{m!} \operatorname{sym}_r^i(\xi_{k-1} - \xi_k, \ldots, \xi_{k-i} - \xi_k) f_b^{(r)}, \tag{10}$$

where $i = 0, \ldots, n$, $n = [m/2]$, $f_a^{(0)} = f_0$, $f_b^{(0)} = f_l$.

Proof The function $\psi_{i,m}$ from (5) can be rewritten in the form

$$\psi_{i,m}(x) = \frac{1}{m!} \operatorname{sym}_m^m(\xi_{i+1} - x, \ldots, \xi_{i+m} - x)$$

and its derivatives are

$$\psi_{i,m}^{(r)}(x) = (-1)^r \frac{r!}{m!} \operatorname{sym}_{m-r}^m(\xi_{i+1} - x, \ldots, \xi_{i+m} - x).$$

Now the de Boor–Fix functionals (4) have the form

$$\lambda_i^m g = \sum_{r=0}^{m} \frac{(m-r)!}{m!} \operatorname{sym}_r^m(\xi_{i+1} - \tau_i, \ldots, \xi_{i+m} - \tau_i) g^{(r)}(\tau_i).$$

Under the action of the de Boor–Fix functionals on the spline s of degree m, we obtain the following set of formulas relating the coefficients of the B-spline expansion and the derivatives of this spline:

$$\alpha_i = \sum_{r=0}^{m} \frac{(m-r)!}{m!} \operatorname{sym}_r^m(\xi_{i+1} - \tau_i, \ldots, \xi_{i+m} - \tau_i) s^{(r)}(\tau_i) \tag{11}$$

for any point τ_i from (ξ_i, ξ_{i+m+1}).

If we take as the point τ_i the extreme knot of the mesh δ, namely $\tau_i = \xi_0$, then the relations (11) can be written for the indices $i = -m, \ldots, 0$. In order to, in the case of multiple additional knots, the point τ_i belongs to (ξ_i, ξ_{i+m+1}), we assume that $\tau_i = \xi_0^+$. Then some arguments of the elementary symmetric functions in (11) will be equal to zero, therefore, using the fact that

$$\operatorname{sym}_r^m(t_1, \ldots, t_{m-1}, 0) = \operatorname{sym}_r^{m-1}(t_1, \ldots, t_{m-1})$$

for $r < m$, the expressions (11) take the form

$$\alpha_i = \sum_{r=0}^{m+i} \frac{(m-r)!}{m!} \operatorname{sym}_r^{m+i}(\xi_1 - \xi_0, \ldots, \xi_{i+m} - \xi_0) s^{(r)}(\xi_0)$$

with $i = -m, \ldots, 0$. In particular, the first coefficient α_{-m} will be equal just to the spline value $s(x_0)$ at the left end of the segment $[a, b]$, the second coefficient α_{-m+1} will be expressed in terms of the spline value and its first derivative

$$\alpha_{-m+1} = s(x_0) + \frac{\xi_1 - \xi_0}{m} s'(x_0)$$

and so on. It is clear that at the right end of the interval $[a, b]$ the situation will be similar, therefore

$$\alpha_{k-1-i} = \sum_{r=0}^{i} \frac{(m-r)!}{m!} \operatorname{sym}_r^{i}(\xi_{k-1} - \xi_k, \ldots, \xi_{k-i} - \xi_k) s^{(r)}(\xi_k)$$

with $i = 0, \ldots, m$. In terms of our interpolation problem,

$$s^{(r)}(x_0) = f_a^{(r)}, \quad s^{(r)}(x_l) = f_b^{(r)}, \quad r = 0, \ldots, n,$$

and $x_0 = \xi_0$, $x_l = \xi_k$. $\qquad\square$

Remark 4.2 The explicit formulas (9) and (10) for splines of odd degree were obtained in [7] without de Boor–Fix functionals.

If we eliminate the obtained parameters $\alpha_{-m}, \ldots, \alpha_{-m+n}$ and $\alpha_{k-1-n}, \ldots, \alpha_{k-1}$ from equations (7) for $i = 1, \ldots, l-1$, to determine the remaining unknowns, which can be written in the form of a vector $\boldsymbol{\alpha} = (\alpha_{-m+n+1}, \ldots, \alpha_{k-n-2})^{\mathrm{T}}$, we obtain a system of $l - 1$ (or $k + m - 2n - 2$) equations

$$A\boldsymbol{\alpha} = \boldsymbol{c}, \tag{12}$$

with the $(l - 1) \times (l - 1)$ matrix

$$A = (N_j(x_i))_{i,j}, \quad i = 1, \ldots, l-1, \quad j = -m+n+1, \ldots, k-2-n,$$

and the vector on the right-hand side $\boldsymbol{c} = (c_1, \ldots, c_{l-1})^{\mathrm{T}}$. The vector on the right-hand side of the system has the following components:

$$c_i = \begin{cases} f_i - \sum\limits_{j=-m+1}^{-m+n} \alpha_j N_j(x_i), & i = 1, \ldots, n, \\ f_i, & i = n+1, \ldots, k-2-n, \\ f_i - \sum\limits_{j=k-1-n}^{k-2} \alpha_j N_j(x_i), & i = k-1-n, \ldots, l-1. \end{cases}$$

The point x_i belongs to supp N_j for $i - m \leqslant j \leqslant i + 2n - m$, hence the matrix A is banded, the band width being equal to $2n + 1$.

Note, if the coefficients of the expansion of any derivative of an interpolating spline in normalized B-splines of a relevant degree are chosen as defining parameters [6,8], such approach of using of de Boor–Fix functionals also makes it possible to obtain explicit formulas for the first and last coefficients.

5 The quartic spline

We end our paper with an example for quartic ($n = 2$, $m = 2n = 4$) splines in Subbotin's scheme. An example of the cubic spline was given in [7].

The interpolated values f_i, $i = 0, \ldots, l$, are given at nodes of the partition Δ: $a = x_0 < x_1 < \cdots < x_l = b$ of the segment $[a, b]$ and the derivatives f'_a, f''_a and f'_b, f''_b at the endpoints of $[a, b]$. The quartic spline s interpolates given values as a spline with knots in the mesh δ: $a = \xi_0 < \xi_1 < \cdots < \xi_k = b$ with $\xi_i = (x_{i-1} + x_i)/2$ and $k = l + 1$.

Let us denote $h_i := x_{i+1} - x_i$, $i = 0, \ldots, l$. In accordance with formulas (9), three parameters at the left end can be determined by the following explicit expressions:

$$\alpha_{-4} = f_a, \qquad \alpha_{-3} = f_a + \frac{h_0}{8} f'_a,$$

$$\alpha_{-2} = f_a + \frac{3h_0 + h_1}{8} f'_a + \frac{h_0(2h_0 + h_1)}{48} f''_a,$$

since $\xi_1 - \xi_0 = h_0/2$, $\xi_2 - \xi_0 = h_0 + h_1/2$. Similar explicit formulas hold also at the right end:

$$\alpha_{l-2} = f_b - \frac{h_{l-1} + 3h_l}{8} f'_b + \frac{h_l(h_{l-1} + 2h_l)}{48} f''_b,$$

$$\alpha_{l-1} = f_b - \frac{h_l}{8} f'_b, \qquad \alpha_l = f_b,$$

with $\xi_{k-1} - \xi_k = h_l/2$, $\xi_{k-2} - \xi_k = h_{l-1}/2 + h_l$. The remaining B-spline coefficients $\alpha_{-1}, \ldots, \alpha_{l-3}$ can be found from the pentadiagonal system of equations (12). Here $N_{-4}, \ldots, N_l$ is the basis of quartic splines on the mesh δ of $[a, b]$.

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