CUBIC SPLINE INTERPOLATION WITH QUASIMINIMAL B-SPLINE COEFFICIENTS

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Abstract. The end conditions for cubic spline interpolation with equidistant knots will be defined so as to make the (slightly modified) B-spline coefficients minimal. This produces good approximation results as compared e.g. with the not-a-knot spline.

1. Introduction

For a natural n let $\Omega_n = \{a + ih, i = 0, ..., n\}$ be an equidistant (uniform) partition of the real interval [a, b] with h = (b - a)/n. Let $S_3(\Omega_n)$ be the linear space of cubic splines with regard to this partition. Any such spline s can be written uniquely as

$$s = \sum_{i=-3}^{n-1} c_i B_{3,i},$$

where $B_{3,i}$ are the cubic B-splines for the extended knot sequence $\Omega_{\infty} = \{x_i = a + ih, i \in \mathbb{Z}\}$. For convenience, we give the derivatives of the B-spline $B_{3,i}$ supported in $[x_i, x_{i+4}]$ at the relevant knots in the following table:

	x_i	x_{i+1}	x_{i+2}	x_{i+3}	x_{i+4}
$B_{3,i}(x)$	0	1/6	2/3	1/6	0
$B_{3,i}'(x)$	0	1/2h	0	-1/2h	0
$B_{3,i}''(x)$	0	$1/h^{2}$	$-2/h^2$	$1/h^2$	0

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Given a real function f defined in [a, b], the interpolatory conditions $s(x_i)$ $= f(x_i), 0 \leq i \leq n$ assume

(1)
$$Mc = \hat{f}$$

where $M = \frac{1}{6}$ tridiag (1, 4, 1) is an $(n+1) \times (n+3)$ matrix, $\hat{f} \equiv f|_{\Omega_n}$ is the column of the function values $(f(x_i))_{i=0}^n$, and c is the column of the unknown coefficients $(c_i)_{i=-3}^{n-1}$. We use the notations of [5], Ch. 6.

Our aim is to fix the two end conditions such that the resulting spline

- minimizes the quadratic sum $||c||^2 = \sum_{i=-3}^{n-1} c_i^2$ of the coefficients, and reproduces the set of cubic polynomials.

Unfortunately, these requirements are conflicting. Hence we will introduce (in the form of a diagonal matrix) further parameters to 'scale down' the B-splines, especially the near-end ones.

The method derived has the optimal order of convergence. To prove this, we make use of the properties of the not-a-knot spline [3], cf. [4]: "(ii) It may be possible to carry out the argument by perturbation, ... showing that the change in the side conditions ... is gentle enough (at least for large n) to change ||P''|| by a bounded amount..."

The new, (quasi)minimal spline will not bear comparison, of course, with splines using derivative information at the ends; however, it proves to be superior to the not-a-knot spline, as numerical tests suggest.

2. Determining the end conditions

Let the additional unknown rows be r_a and r_b , where the subscripts indicate that they are related to a and b. Then we get the enlarged system

(2)
$$\begin{pmatrix} r_a \\ M \\ r_b \end{pmatrix} c = \begin{pmatrix} 0 \\ \hat{f} \\ 0 \end{pmatrix}$$

of linear equations with a square matrix.

Our first statement concerns the problem of minimality.

LEMMA 1. The solution c of (2) is the minimal solution of (1) if and only if r_a and r_b are linearly independent and are orthogonal to the rows of M, i.e.

$$r_a M^T = 0, \qquad r_b M^T = 0.$$

A possible solution for this is

(3)
$$r_a = (1, \lambda_1, \lambda_1^2, \dots, \lambda_1^{n+2}), \quad r_b = (\lambda_1^{n+2}, \dots, \lambda_1^2, \lambda_1, 1)$$

with $\lambda_1 = -2 + \sqrt{3}$.

PROOF. As for the first part, it is enough to note that the minimal solution for (1) is given by

$$M^+\hat{f} = M^T (MM^T)^{-1}\hat{f},$$

where M^+ stands for the Moore–Penrose pseudoinverse of M.

To prove (3), consider the homogeneous linear system $rM^T = 0$ as a recursion for r with characteristic polynomial $\lambda^2 + 4\lambda + 1$. Its zeros are λ_1 and $\lambda_2 = 1/\lambda_1$, hence r_a is appropriate, and so is r_b , for it is a scalar multiple of $(1, \lambda_2, \lambda_2^2, \ldots, \lambda_2^{n+2}).$

COROLLARY. Let us insert a diagonal positive definite matrix D_0 in the linear systems (1-2) to get the pair

$$(MD_0^{-1})(D_0)c = \hat{f} \quad and \quad \begin{pmatrix} r_a D_0 \\ MD_0^{-1} \\ r_b D_0 \end{pmatrix} (D_0c) = \begin{pmatrix} 0 \\ \hat{f} \\ 0 \end{pmatrix}$$

If r_a and r_b are chosen according to (3), then the solution of the second is the minimal solution of the first equation – irrespective of D_0 ! This follows from $(rD_0)(MD_0^{-1})^T = rM^T$, with $r = r_a$ and $r = r_b$.

REMARKS. 1. The spline obtained in this way is called quasiminimal because of the presence of D_0 : note that in fact $||D_0c||$ will be minimal.

2. The notation can be simplified by introducing $D = D_0^2$. With this, our system takes the form

(4)
$$\begin{pmatrix} r_a D \\ M \\ r_b D \end{pmatrix} c = \begin{pmatrix} 0 \\ \hat{f} \\ 0 \end{pmatrix}.$$

,

Thus, assuming r_a and r_b are the rows in (3), quasiminimality is assured, and we only have to care for the reproducing property.

3. Observe that r_b is the reverse of r_a , or, by help of the so-called backward identity J (where the ones lie on the secondary diagonal), $r_b = r_a J$ holds. We want to maintain this kind of symmetry for D as well, by requiring D = JDJ, i.e. DJ = JD. Such matrices are called persymmetric; in our case we simply have

$$D = \operatorname{diag}(d_i), \quad d_i = d_{n+4-i}, \quad 1 \leq i \leq n+3.$$

LEMMA 2. Let D be a positive definite persymmetric diagonal matrix, and r_a and r_b be such that the matrix on the left of (4) is invertible. Then the spline calculated on the basis of (4) is reproducing if and only if

(5)
$$r_a D e^{(j)} = 0, \qquad 0 \le j \le 3,$$

where $e^{(j)} = (0^j, 1^j, \dots, (n+2)^j)^T$.

PROOF. The necessity follows from the unique representation of id^j in the form

$$\operatorname{id}^{j} = \sum_{i=-3}^{n-1} p_{j}(i) B_{3,i},$$

with p_j a *j*-th degree polynomial, $0 \leq j \leq 3$. To prove sufficiency, first we show that (5) holds with r_a replaced by r_b , too.

The case j = 0 is evident. If j = 1, then $r_b De^{(1)} = r_a J De^{(1)} = r_a D J e^{(1)}$, where $Je^{(1)}$ is a linear combination of $e^{(0)}$ and $e^{(1)}$, hence $r_b De^{(1)} = 0$. Continuing this way, we get $r_b De^{(j)} = 0$, $0 \leq j \leq 3$. The rest follows by the fact that the solution of (4) is unique.

REMARK. Since (5) represents only four equations, the majority of the d_i -s can be fixed:

(6)
$$d_i = 1, \qquad 5 \leq i \leq n-1.$$

Assuming now (3), (6), and persymmetry for D, (5) can be solved for any $n \ge 6$. We obtain e.g.

$$d_1 = \frac{1}{454}, \quad d_2 = \frac{8}{227}, \quad d_3 = \frac{50}{227}, \quad d_4 = \frac{152}{227}$$

for n = 6, and

$$d_1 = \frac{1}{758}, \quad d_2 = \frac{17}{758}, \quad d_3 = \frac{58}{379}, \quad d_4 = \frac{202}{379}$$

for n = 7.

It is worth calculating the limits of these parameters for the sake of the convergence proof, for stability reasons, and also since their first 15 digits are, starting from n = 36, unchanged. Note that, in fact, $d_i = d_i^{(n)}$.

LEMMA 3. Denote $d_i^* = \lim_{n \to \infty} d_i$, $1 \leq i \leq 4$. We have

(7)
$$d_1^* = \frac{7 - 4\sqrt{3}}{36}, \quad d_2^* = \frac{15 - 8\sqrt{3}}{36}, \quad d_3^* = \frac{21 - 8\sqrt{3}}{36}, \quad d_4^* = \frac{29 - 4\sqrt{3}}{36}$$

with $d_i - d_i^* = O(\lambda_1^n), \ \lambda_1 = -2 + \sqrt{3}.$

PROOF. We only display the system (5) to be solved, using matrix formalism. Let M_a be the Vandermonde matrix with second generating row (0, 1, 2, 3), i.e. let

$$M_a = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 1 & 4 & 9 \\ 0 & 1 & 8 & 27 \end{pmatrix}$$

let M_b be the Vandermonde matrix with second row (n+2, n+1, n, n-1), define matrices $\Lambda_a = \text{diag}(1, \lambda_1, \lambda_1^2, \lambda_1^3)$, $\Lambda_b = \text{diag}(\lambda_1^{n+2}, \lambda_1^{n+1}, \lambda_1^n, \lambda_1^{n-1})$, introduce the column vector

rhs =
$$-\left(\sum_{i=4}^{n-2} t^i, \sum_{i=4}^{n-2} it^i, \sum_{i=4}^{n-2} i^2 t^i, \sum_{i=4}^{n-2} i^3 t^i\right)^T$$
,

and the unknown column $d = (d_i)_{i=1}^4$. Then (5) is equivalent with

(8)
$$(M_a\Lambda_a + M_b\Lambda_b) d = \text{rhs}.$$

Focusing now on determining the limit values (d_i^*) , the second matrix $M_b \Lambda_b$ can be omitted, and the right hand vector rhs also simplifies to

rhs^{*} =
$$-\lambda_1^4 \mu_1 \begin{pmatrix} 1 \\ \mu_1(4 - 3\lambda_1) \\ \mu_1^2(16 - 23\lambda_1 + 9\lambda_1^2) \\ \mu_1^3(64 - 131\lambda_1 + 100\lambda_1^2 - 27\lambda_1^3) \end{pmatrix}$$

with $\mu_1 = (1 - \lambda_1)^{-1}$. Now we have the simpler system $M_a \Lambda_a d^* = \text{rhs}^*$, with the solution stated.

The order of convergence follows from the standard estimation for linear systems ([8], [5]):

$$\frac{\|\Delta x\|}{\|x\|} \leq \frac{\kappa(A)}{1 - \kappa(A) \frac{\|\Delta A\|}{\|A\|}} \left(\frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta b\|}{\|b\|} \right), \quad \kappa(A) = \|A\| \, \|A^{-1}\|$$

applied to $A = M_a \Lambda_a$, $x = d^*$, $b = \text{rhs}^*$, $\Delta A = M_b \Lambda_b$, $\Delta b = \text{rhs} - \text{rhs}^*$. Since both $\|\Delta A\| = O(\lambda_1^n)$ and $\|\Delta b\| = O(\lambda_1^n)$, the denominator on the right of the inequality, $1 - \|A^{-1}\| \|\Delta A\|$ is positive for *n* large enough, showing that the perturbed matrix is also invertible and the estimate holds. Note finally that, using 2-norm (i.e. operator norm), $\kappa(M_a\Lambda_a) = 54.4587$.

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REMARKS. 1. The limit values (d_i^*) can be checked by the Inverse Symbolic Calculator [6] on the internet; calculating the d_i -s from (8) for n large $(n \ge 36)$, the program recognizes the irrational values (7).

2. Using the limits (d_i^*) instead of the values (d_i) , the resulting spline is, of course, only asymptotically reproducing with indicated error $O(\lambda_1^n)$.

3. The case of quadratic splines has been handled in [7], where the matrix M was $(n + 1) \times (n + 2)$, and there were only two scaling parameters: α_n and β_n . In the present notation they are d_1 and d_2 with limits $\frac{1}{4}$ and $\frac{3}{4}$.

3. The convergence

To prove convergence, we will exploit the same property of the not-a-knot spline, the definition of which requires the third derivative to be continuous across x_1 and x_{n-1} . As the following table shows, we use overlined variables for the not-a-knot spline, to distinguish between the two kinds of splines:

	first row	last row	coef	spline
Not-a-knot	\overline{r}_a	\overline{r}_b	\overline{c}	\overline{s}
Quasiminimal	$r_a D$	$r_b D$	c	s

Thus, using equally spaced knots we have

$$\overline{r}_a = (1, -4, 6, -4, 1, 0, \dots 0), \qquad \overline{r}_b = \overline{r}_a J$$

the end-conditions assume $\overline{r}_a \overline{c} = 0$, $\overline{r}_b \overline{c} = 0$, and the not-a-knot spline has the representation $\overline{s} = \sum_{i=-3}^{n-1} \overline{c}_i B_{3,i}$ on [a, b]. Observe that \overline{r}_a and \overline{r}_b are special cases of the rows

$$\bar{r}_i = (0, \dots, 0, 1, -4, 6, -4, 1, 0, \dots, 0),$$

with the trailing '1' in the i-th position.

Our last perparatory lemma concerns the connection of both methods.

LEMMA 4. The system

$$\sum_{i=1}^{n-1} t_i \overline{r}_i = \frac{1}{d_i} r_a D$$

of linear equations with (3-6) holding is consistent with solution

$$t_i = \lambda_1^{i-1} + O(\lambda_1^n), \qquad \lambda_1 = -2 + \sqrt{3}.$$

PROOF. The Kronecker–Kapelli theorem tells us that $r_a D$ is a linear combination of the \overline{r}_i -s if and only if $r_a D$ is orthogonal to the subspace H of all rows, orthogonal to the \overline{r}_i -s. To find a basis in H, take the characteristic equation $(\mu - 1)^4 = 0$ of this homogeneous recursion. Its solution $\mu_1 = 1$ is of multiplicity 4, giving the basis

$$\{\mu_1^i,\ i\mu_1^i,\ i^2\mu_1^i,\ i^3\mu_1^i\}=\{1,\ i,\ i^2,\ i^3\}$$

for *H*. However, this is exactly the set $(e^{(j)})_{j=0}^3$, therefore solvability is guaranteed, cf. (5). As regards the form of the solution *t*, we replace d_i by d_i^* , $i = 1, \ldots, 4$ and distinguish three cases.

a) The majority – the 'middle' – of the equations has the form

$$t_{i-4} - 4t_{i-3} + 6t_{i-2} - 4t_{i-1} + t_i = \frac{1}{d_i^*} \lambda_1^{i-1}, \qquad 5 \le i \le n-5,$$

where the right hand side can be written as $36\lambda_1^{i-3}$, due to the immediately calculated equality $\lambda_1^2 = 36d_1^*$. The trial $t_i = \lambda_1^{i-1}$ gives now $(\lambda_1 - 1)^4 = 36\lambda_1^2$, which is true owing to the factorization

$$(\lambda - 1)^4 - 36\lambda^2 = (\lambda^2 + 4\lambda + 1)(\lambda^2 - 8\lambda + 1)$$

and the fact that $\lambda_1^2 + 4\lambda_1 + 1 = 0$.

b) The first four equations can immediately be verified to be true:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ -4 & 1 & 0 & 0 \\ 6 & -4 & 1 & 0 \\ -4 & 6 & -4 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ \lambda_1 \\ \lambda_1^2 \\ \lambda_1^3 \end{pmatrix} = \frac{1}{d_1^*} \begin{pmatrix} d_1^* \\ \lambda_1 d_2^* \\ \lambda_1^2 d_3^* \\ \lambda_1^3 d_4^* \end{pmatrix}.$$

c) The last four equations are false either with d_i -s or with d_i^* -s, however, both sides are within $O(\lambda_1^n)$.

THEOREM. For the quasiminimal spline s defined by (2) to (6) it holds that

$$f - s = O(h^4), \qquad f \in \mathbf{C}^4[a, b],$$

PROOF. We know that the not-a-knot spline \overline{s} satisfies $f - \overline{s} = O(h^4)$. By the triangle inequality we have

$$||f - s|| \leq ||f - \overline{s}|| + ||\overline{s} - s||$$

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for the uniform norm, thus it suffices to investigate the difference $\overline{s} - s$ of the not-a-knot and quasiminimal splines. Since both of them satisfy the interpolatory conditions, their difference vanishes at the knots, and the homogeneous system $M(\overline{c} - c) = 0$ holds for the difference of the coefficients for the B-spline representations. Thus, $\overline{c} - c$ belongs to the two-dimensional subspace generated by r_a^T and r_b^T , i.e.

$$\overline{c} - c = \alpha r_a^T + \beta r_b^T$$

Multiplying by $r_a D$ and $r_b D$, resp., and using the definition

$$r_a Dc = 0, \qquad r_b Dc = 0$$

of quasiminimal splines, we obtain

$$\begin{pmatrix} r_a D r_a^T & r_a D r_b^T \\ r_b D r_a^T & r_b D r_b^T \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} r_a D \overline{c} \\ r_b D \overline{c} \end{pmatrix}.$$

The Gramian on the left can be calculated to tend to δI_2 , a scalar multiple of the identity with $\delta = \frac{13}{\sqrt{3}} - \frac{15}{2} \approx 0.0055$. Hence it is enough to estimate the right hand vector. Since both coordinates are handled equally, we take $r_a D\bar{c}$, and apply Lemma 4 to get

$$r_a D\overline{c} = \sum_{i=1}^{n-1} t_i \overline{r}_i \overline{c}$$
 with $t_i = \lambda_1^{i-1} + O(\lambda_1^n).$

Here $\bar{r}_1 \bar{c} \equiv \bar{r}_a \bar{c} = 0$, $\bar{r}_{n-1} \bar{c} \equiv \bar{r}_b \bar{c} = 0$ by definition of the not-a-knot spline. For the remaining terms we have

$$\overline{r}_{i}\overline{c} = \overline{c}_{i-4} - 4\overline{c}_{i-3} + 6\overline{c}_{i-2} - 4\overline{c}_{i-1} + \overline{c}_{i}$$
$$= h^{2} \left(\overline{s}''(x_{i+1}) - 2\overline{s}''(x_{i}) + \overline{s}''(x_{i-1})\right)$$
$$= 6h^{2} \left(\frac{f(x_{i+1}) - 2f(x_{i}) + f(x_{i-1})}{h^{2}} - \overline{s}''(x_{i})\right)$$

due to the representations

$$s(x_j) = \frac{1}{6} \left(c_{j-3} + 4c_{j-2} + c_{j-1} \right), \quad s''(x_j) = \frac{1}{h^2} \left(c_{j-3} - 2c_{j-2} + c_{j-1} \right),$$

and the identity

(9)
$$\frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} = \frac{\overline{s}''(x_{i-1}) + 4\overline{s}''(x_i) + \overline{s}''(x_{i+1})}{6}$$

Since $\frac{1}{h^2} (f(x_{i+1}) - 2f(x_i) + f(x_{i-1})) - f''(x_i) = O(h^2)$ by the assumption on f, and $f''(x_i) - \overline{s}''(x_i) = O(h^2)$ by the known property of the not-a-knot spline, we conclude that $\overline{r}_i \overline{c} = O(h^4)$. Consequently, $\overline{c} - c = O(h^4)$ and we have for all $x \in [a, b]$

$$\left|\overline{s}(x) - s(x)\right| \leq \max \left|\overline{c}_i - c_i\right| \cdot \left|\sum_{i=-3}^{n-1} B_{3,i}(x)\right|,$$

i.e.

$$\|\overline{s} - s\|_{C[a,b]} \leq \|\overline{c} - c\|_{\infty} = O(h^4)$$

by the partition of unity for B-splines. This completes the proof.

REMARKS. 1. Identity (9) is interesting in itself: it is true for any interpolation spline – irrespective of the two additional conditions. It can be found in [1] as well, in a more general context.

2. There is another natural (not minimal) choice for the supplementary conditions. Disregard to this the settings (6) and choose

$$\varrho_a = \left(\binom{n+1}{0}, \binom{n+1}{1}, \dots, \binom{n+1}{n+1}, 0 \right), \qquad \varrho_b = \varrho_a J$$

instead. One attains this by considering the last two columns of the inverse Vandermonde matrix, resulting in $\rho_a e^{(j)} = 0$, $0 \leq j \leq 3$, a condition for reproducibleness, cf. (5). Applied to a k-th degree polynomial $f, k \leq n + 1$, the coefficients c_i obtained here also are k-th degree polynomials of their subscript. This method is favourable for analytical functions, however fails to converge for functions of the class $C^4[a, b]$, by the analogy with Lagrange interpolation.

4. Numerical tests

The following notations will be used. The quasiminimal spline with scaling factors (d_i) and their limits (d_i^*) -s will be denoted by QM and QM^* , resp. The above mentioned method with 'polynomial coefficients' will be referred to as method PC, and (n - a - kn) will stand for the not-a-knot spline. Then we have the following list of C[a, b] errors; notice that the common factor γ is picked out for brevity. Further, Runge $(x) = 1/(1 + x^2)$, and the MATLAB conventions are used.

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$\int f$	[a,b]	n	γ	QM	QM^*	PC	n-a-kn
id^4	[0,1]	10	1e - 5	5.1	5.4	0.6	6.8
id^4	[0, 1]	20	1e - 6	3	3	0.3	4.2
atan	[0,5]	10	1e - 3	5.1	5.1	1.4	5.6
atan	[0, 5]	20	1e - 3	0.34	0.34	0.06	0.48
atan	[-5, 5]	10	1e - 2	2.9	2.9	21	2.9
atan	[-5, 5]	20	1e - 3	1.8	1.8	795	1.8
Runge	[-5, 5]	10	1e - 2	2.2	2.2	174	2.2
Runge	[-5, 5]	20	1e - 3	3.2	3.2	1e4	3.2
abs	[-1, 1]	10	1e - 2	3.4	3.4	61	3.39
abs	[-1, 1]	20	1e - 2	1.7	1.7	2e3	1.7
exp	[0, 1]	10	1e - 5	0.5	5	0.07	0.7
exp	[0, 1]	20	1e - 7	3.3	3.3	0.4	4.5
tan	[-1.5, 1.5]	10	1	2.72	2.71	1.9	2.8
tan	[-1.5, 1.5]	20	1e - 5	1.24	1.24	0.57	1.3
sin	$\left[-\frac{5\pi}{2},\frac{5\pi}{2}\right]$	10	1e-2	2.52	2.85	39	2
sin	$\left[-\frac{5\pi}{2},\frac{5\pi}{2}\right]$	20	1e-3	6.4	6.4	1.1	7.3

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