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Optimal Interpolatory Splines Using B-spline Representation

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Abstract

The natural splines of odd degree $2m-1$ interpolating given data are known to have a minimal L_2-norm of its m-th derivative on the class of interpolants from W_2^m. Similarly the natural splines of even degree $2m$ interpolating mean values are known to have a minimal L_2-norm of its m-th derivative on the class of interpolants from W_2^m. In this paper we will consider the class of interpolatory splines of degree $k>0$ only and we will use free parameters of such interpolatory splines of degree $k>0$ to minimize some functionals with geometrical or physical meaning (curvature, energy). To get this spline we shall use the B-spline basis and a minimum N-(semi)norm g-inverse of some matrix.

Key words: Interpolatory spline, norm optimization, B-spline basis, minimum N-(semi)norm g-inverse of matrix.

2000 Mathematics Subject Classification: 65F20, 65D05, 65D07

1 Introduction

Let the sequence of knots $\Delta\lambda := \lambda_1 < \ldots \lambda_g$, $a < \lambda_j < b$, $j = 1, \ldots, g$ and the prescribed data (x_i, y_i), $a \le x_i \le b$, $i = 1, \ldots, n$ be given. In this paper we will consider the vector space of splines of degree $k > 0$, defined on an interval $[a, b]$ with the sequence of knots $\Delta\lambda$. Our problem is to find a spline of degree $k > 0$

interpolating data (x_i, y_i), $i = 1, \ldots, n$, and minimizing some functionals with geometrical or physical meaning. In the following this spline will be referred as *an optimal interpolatory spline.*

We shall give the conditions under which the optimal interpolatory spline of degree $k > 0$ exists and it is unique.

The problem of the optimal interpolation *Let the sequence of knots $\Delta\lambda$ and data (x_i, y_i), $a \le x_i \le b$, $i = 1, \ldots, n$ be given. The problem is to find a spline $s_k(x)$ of degree $k > 0$, defined on interval $[a, b]$, with the knots $\Delta\lambda$, interpolating data (x_i, y_i), $i = 1, \ldots, n$ for which*

$$J_l(s_k) = \int_a^b \left[s_k^{(l)}(x)\right]^2 dx, \quad l \in \{0, 1, \ldots, k-1\} \tag{1}$$

is minimal.

We will use the B-spline representation of the spline, which will be described in the following section.

2 The B-spline representation

The vector space of splines of degree $k > 0$, defined on interval [a,b], with the knots $\Delta\lambda$, will be denoted by $\mathcal{S}_k[a, b]$. Its dimension is

$$\dim(\mathcal{S}_k[a, b]) = g + k + 1.$$

Every spline $s_k(x) \in \mathcal{S}_k[a, b]$ can be written as a unique linear combination of some $g + k + 1$ basis function. We will consider the B-spline basis. To obtain this basis we need additional knots

$$\lambda_{-k} \le \ldots \le \lambda_{-1} \le \lambda_0 = a \quad \text{and} \quad b = \lambda_{g+1} \le \lambda_{g+2} \le \ldots \le \lambda_{g+k+1}.$$

With these additional knots we can construct the B-spline basis $\left\{B_i^{k+1}\right\}_{i=-k}^{g}$ and every spline $s_k(x) \in \mathcal{S}_k[a, b]$ has a unique representation

$$s_k(x) = \sum_{i=-k}^{g} b_i B_i^{k+1}(x), \tag{2}$$

where b_i are called *the B-spline coefficients of $s_k(x)$.*

Now let $\mathcal{M}_{m,n}$ denotes a set of (m, n) matrices and $\mathcal{M}_n = \mathcal{M}_{n,n}$. Further we will use *a collocation matrix* $C_{k+1}(x)$ for a given vector $x = (x_1, \ldots, x_n)^T$. The following definition was published in [1].

Definition 2.1 Let $x \in \mathcal{M}_{n,1}$. *The collocation matrix* $C_{k+1}(x) \in \mathcal{M}_{n,g+k+1}$ of B-splines $B_i^{k+1}(x)$, $i = -k, \ldots, g$ for a vector $x = (x_1, \ldots, x_n)^T$ is defined as

$$C_{k+1}(x) = \begin{pmatrix} B_{-k}^{k+1}(x_1) & \ldots & B_g^{k+1}(x_1) \\ \vdots & \ddots & \vdots \\ B_{-k}^{k+1}(x_n) & \ldots & B_g^{k+1}(x_n) \end{pmatrix}. \tag{3}$$

The following theorem states basic properties of the collocation matrix $C_{k+1}(x)$.

Theorem 2.2 (Schoenberg–Whitney conditions, see [1], [3]) *Let $x \in \mathcal{M}_{n,1}$. Then for the matrix $C_{k+1}(x)$ the following statements hold.*

a) $C_{k+1}(x)$ is of full column rank if and only if $n > g+k+1$ and there exists $\{u_{-k},\dots,u_g\} \subset \{x_1,\dots,x_n\}$ with $u_i < u_{i+1}$, $i=-k,\dots,g-1$ such that

$$\lambda_i < u_i < \lambda_{i+k+1}, \quad i=-k,\dots,g.$$

b) $C_{k+1}(x)$ is regular if and only if

$$n = g+k+1 \qquad \text{and} \qquad \lambda_{i-k-1} < x_i < \lambda_i, \quad i=1,\dots,n.$$

c) $C_{k+1}(x)$ is of full row rank if and only if $n < g+k+1$ and there exists $\{\mu_1,\dots,\mu_n\} \subset \{\lambda_{-k},\dots,\lambda_g\}$ with $\mu_i < \mu_{i+1}$, $i=1,\dots,n-1$ such that

$$\mu_i < x_i < \mu_{i+k+1}, \quad i=1,\dots,n.$$

For $l \in \{1,\dots,k-1\}$, the l-th order derivative of a spline $s_k(x)$ of degree $k>0$ is a spline of degree $k-l$ having the same knots. Its B-spline coefficients can be easily computed from those of $s_k(x)$, i.e.

$$s_k^{(l)}(x) = \prod_{j=1}^{l}(k+1-j) \sum_{i=-(k-l)}^{g} b_i^{(l)} B_i^{k+1-l}(x), \tag{4}$$

with

$$b_i^{(j)} = \begin{cases} b_i & \text{if } j=0, \\ \dfrac{b_i^{(j-1)} - b_{i-1}^{(j-1)}}{\lambda_{i+k+1-j} - \lambda_i} & \text{if } j>0. \end{cases} \tag{5}$$

For more details see in [3]. In matrix notation we can write

$$s_k^{(l)}(x) = \prod_{j=1}^{l}(k+1-j) C_{k+1-l}(x) b^{(l)}, \tag{6}$$

where

$$b^{(l)} = S_l b, \qquad \text{with } S_l = D_l L_l \dots D_1 L_1 \in \mathcal{M}_{g+k+1-l,g+k+1}, \tag{7}$$

and with

$$D_j := diag\left(\frac{1}{\lambda_{i+k+1-j} - \lambda_i}\right)_{i=-(k-j),\dots,g} \in \mathcal{M}_{g+k+1-j}$$

and bidiagonal matrix

$$L_j := \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix} \in \mathcal{M}_{g+k+1-j,g+k+2-j}.$$

3 g-inverse for a minimum norm solution of a consistent system $Ax = z$

Consider the system of linear equations

$$Ax = z. \tag{8}$$

If $A \in \mathcal{M}_m$ is nonsingular matrix and $z \in \mathcal{M}_{m,1}$, the unique solution of the linear equation (8) is given by $x = A^{-1}z$. In this section we consider a general matrix $A \in \mathcal{M}_{m,n}$ and vector $z \in \mathcal{M}_{m,1}$ and we want to describe all solutions of the system of linear equations (8).

If there exists a matrix G such that $x = Gz$ is a solution of (8) for any z such that $Ax = z$ is a consistent equation, then G does the same job as the inverse A^{-1} of A, hence may be called *a generalized inverse (g-inverse) of A* and it is denoted by A^-. For general matrix $A \in \mathcal{M}_{m,n}$ the g-inverse A^- is not unique. If A is nonsingular matrix, then $A^- = A^{-1}$.

Theorem 3.1 *Let A^- be a g-inverse of A. Then it is necessary and sufficient that*

$$AA^-A = A.$$

Proof See [9].

Lemma 3.2 *A g-inverse A^- of $A \in \mathcal{M}_{m,n}$ exists and* $\operatorname{rank}(A^-) \geq \operatorname{rank}(A)$.

Proof It is given in [9], pp. 21 and it is based on a rank factorization.

Theorem 3.3 Computation of A^-. *Let $A \in \mathcal{M}_{m,n}$ be a matrix of rank r and let it be possible to rearrange the columns of A in the form $A = (B_1, B_2)$, where $B_1 \in \mathcal{M}_{m,r}$ is of rank r and $B_2 \in \mathcal{M}_{m,n-r}$. Then one choice of g-inverse of A is*

$$A^- = \begin{pmatrix} P \\ 0 \end{pmatrix} \quad \textit{where} \quad P = (B_1^T B_1)^{-1} B_1^T.$$

Proof See [9].

Remark 3.4 In programme system MATLAB we can compute one choice of A^- by MATLAB command *pinv*. Another choice of A^- can be generated by left division operator

$$A^- = A \backslash I_m = A \backslash eye(m). \tag{9}$$

Theorem 3.5 *Let $A \in \mathcal{M}_{m,n}$, any g-inverse A^- of A and an arbitrary vector $u \in \mathcal{M}_{n,1}$ be given. Then*

$$x = A^-z + (I - A^-A)u \tag{10}$$

is a general solution of a consistent nonhomogenous equation $Ax = z$.

Proof See in [9], pp. 24.

Corollary 3.6 *Let $A \in \mathcal{M}_{m,n}$ with $rank(A) = m$, $Z \in \mathcal{M}_{n,n-m}$ such that $AZ = 0$, $rank([A^T, Z]) = n$ and an arbitrary vector $v \in \mathcal{M}_{n-m,1}$ be given. Then*

$$x = A^- z + Zv \tag{11}$$

is a general solution of a consistent nonhomogenous equation $Ax = z$.

Proof a) Every $x = A^- z + Zv$ for an arbitrary vector v is solution of $Ax = z$ because $Ax = AA^- z + AZv = AA^- z = z$. The last equality is easy to verify. Because $Ax = z$ is consistent, we have $z = Aw$ for some vector w and $AA^- Aw = Aw = z$.

b) Let $u = Zv$, where v is an arbitrary vector. Then with respest to the Theorem 3.5 vector $x = A^- z + (I - A^- A)u$ is a solution of $Ax = z$ and $x = A^- z + (I - A^- A)Zv = A^- z + Zv$. $\square$

Let $N \in \mathcal{M}_n$ be a p.d. (positive definite) or p.s.d. (positive semidefinite) matrix. For a vector $u \in \mathcal{M}_{n,1}$ we define the N-norm or N-seminorm $\| u \|_N$ by $\|u\|_N = \sqrt{u^T N u}$ and denote the inner product of two vectors $u, v \in \mathcal{M}_{n,1}$ by $(u, v)_N = v^T N u$.

Now we inquire whether there exists a g-inverse G such that Gz has the smallest N-norm or N-seminorm in the class of all solutions of $Ax = z$, that is, we wish to find a solution of linear equations (8), such that

$$\min_{Ax=z} \|x\|_N = \|Gz\|_N$$

where N is p.d. or p.s.d. matrix. This solution is reffered to as *a minimum N-(semi)norm solution of $Ax = z$.*

Theorem 3.7 *Let G be a g-inverse of A such that Gz is a minimum N-(semi)norm solution of a consistent nonhomegenous equation $Ax = z$. Then it is necessary and sufficient that*

$$AGA = A \qquad (GA)^T N = NGA.$$

Proof See in [9], pp. 44–46.

Remark 3.8 A matrix G which provides the minimum N-(semi)norm solution of $Ax = z$ is denoted A_m^- or more explicitly by $A_{m(N)}^-$ and reffered to as *minimum N-norm or N-seminorm g-inverse of A.* We must note that $A_{m(N)}^-$ may not be unique.

Theorem 3.9 *Let $A \in \mathcal{M}_{m,n}$ be a matrix with $rank(A) = m$, $Z \in \mathcal{M}_{n,n-m}$ be a matrix such that $AZ = 0$, $rank([A^T, Z]) = n$ and $N \in \mathcal{M}_n$ be p.d. or p.s.d. matrix. Then there exists just one minimum N-(semi)norm solution of a consistent nonhomogenous equation $Ax = z$ if and only if $Z^T N Z$ is p.d.*

Proof a) Let $x_0 = Gz$ be a minimum N-(semi)norm solution. Then using Theorem 3.7. is $AGA = A$ and $(GA)^T N = NGA$. A general solution of $Ax = z$ is $x = Gz + Zv$, where $v \in \mathcal{M}_{n-m,1}$ is an arbitrary vector, (see (11) in Corollary 3.6). Now

$$\|x\|_N^2 = \|Gz + Zv\|_N^2 = \|Gz\|_N^2 + 2(Gz, Zv)_N + \|Zv\|_N^2$$

and

$$(Gz, Zv)_N = (Gz, (I - GA)Zv)_N.$$

Because $Ax = z$ is consistent, we have $z = Aw$ for an arbitrary $w \in \mathcal{M}_{n,1}$ and

$$\begin{aligned}(Gz, Zv)_N &= (GAw, (I - GA)Zv)_N = w^T (GA)^T N (I - GA) Zv \\ &= w^T (NGA - NGA) Zv = 0.\end{aligned}$$

Thus we have

$$\|x\|_N^2 = \|Gz\|_N^2 + \|Zv\|_N^2 = \|x_0\|_N^2 + \|Zv\|_N^2.$$

So we can see that $\|x_0\|_N \leq \|x\|_N$. Hence $\|x_0\|_N < \|x\|_N$ if and only if

$$\|Zv\|_N > 0 \Leftrightarrow \|v\|_{Z^T N Z} > 0 \Leftrightarrow Z^T N Z \quad \text{is p.d.}$$

b) Uniqueness: Let $x_0 = G_0 z$ and $x_1 = G_1 z$, where G_0 and G_1 are both $A^-_{m(N)}$ such that $G_0 \neq G_1$ and $\|x_0\|_N = \|x_1\|_N$. Then

$$x_0^T N x_0 - x_1^T N x_1 = 0 \Rightarrow z^T G_0^T N G_0 z - z^T G_1^T N G_1 z = 0.$$

Because $Ax = z$ is consistent, we have $z = Aw$ for an arbitrary $w \in \mathcal{M}_{n,1}$ and

$$\begin{aligned}0 &= z^T G_0^T N G_0 z - z^T G_1^T N G_1 z = w^T A^T G_0^T N G_0 A w - w^T A^T G_1^T N G_1 A w \\ &= w^T \left[(G_0 A)^T N G_0 A - (G_1 A)^T N G_1 A\right] w = w^T \left[N G_0 A - N G_1 A\right] w \\ &\Leftrightarrow N(G_0 - G_1)A = 0\end{aligned}$$

or GA is unique and hence $Gy = GAw$ is unique and hence $x_0 = x_1$. Thus the proof is finished. □

Theorem 3.10

1. Let N be a p.d. matrix. Then one choice of $A^-_{m(N)}$ is

$$N^{-1} A^T (A N^{-1} A^T)^-.$$

2. Let N be a p.s.d matrix. Then one choice of $A^-_{m(N)}$ is

$$(N + A^T A)^- A^T [A(N + A^T A)^- A^T]^-.$$

3. Let N be a p.d. or p.s.d. matrix and let

$$\begin{pmatrix} N & A^T \\ A & 0 \end{pmatrix}^- = \begin{pmatrix} C_1 & C_2 \\ C_3 & C_4 \end{pmatrix}.$$

Then C_2 is minimum N-(semi)norm g-inverse of A.

Proof Proof is given in [9], pp. 45–47.

4 Problem of the optimal interpolation

4.1 The interpolatory conditions

With the given sequence of knots $\Delta\lambda$ and given data (x_i, y_i), $a \le x_i \le b$, $i = 1, \dots, n$ we want to find an interpolatory spline $s_k(x)$ of degree $k > 0$ defined on interval $[a, b]$, which minimizes functional (1). Using the B-spline representation (2) we can rewrite the interpolatory conditions $s_k(x_i) = y_i$, $i = 1, \dots, n$ as

$$s_k(x_i) = \sum_{j=-k}^{g} b_j B_j^{k+1}(x_i) = y_i, \quad i = 1, \dots, n. \tag{12}$$

Relation (12) can be written in matrix notation as

$$C_{k+1}(x) b = y \tag{13}$$

where $b = (b_{-k}, \dots, b_g)^T, y = (y_1, \dots, y_n)^T$ and $C_{k+1}(x) \in \mathcal{M}_{n,g+k+1}$ is collocation matrix (see Definition 2.1).

Now let us discuss the system of linear equations (13) with respect to the knots.

a) If the system (13) is inconsistent, then the optimal interpolatory spline $s_k(x)$ does not exist.

b) If the system (13) is consistent and the matrix $C_{k+1}(x)$ is regular, i.e. (using Theorem 2.2) $n = g + k + 1$ and $\lambda_{i-k-1} < x_i < \lambda_i$, $i = 1, \dots, n$, then there exists just one solution of (13) and there are no free parameters which could be used to the minimization of the functional (1).

c) If the system (13) is consistent and the matrix $C_{k+1}(x)$ is of full row rank, i.e. (using Theorem 2.2) $n < g + k + 1$ and there exists $\{\mu_1, \dots, \mu_n\} \subset \{\lambda_{-k}, \dots, \lambda_g\}$ with $\mu_i < \mu_{i+1}$, $i = 1, \dots, n-1$ such that

$$\mu_i < x_i < \mu_{i+k+1}, \quad i = 1, \dots, n,$$

then there exists a solution of (13) and there are $g + k + 1 - n$ free parameters which we can use to the optimization purposes.

From now we will suppose that we have such sequence of knots $\Delta\lambda$ and such data (x_i, y_i) $i = 1, \dots, n$ that the case c) holds.

4.2 Functional J_l as a seminorm of B-spline coefficients

In this section we rewrite functional $J_l(s_k)$ as a (semi)norm of B-spline coefficients. If we use the B-spline representation (2) and relation (4) then

$$J_l(s_k) = \int_a^b \left[s_k^{(l)}(x) \right]^2 dx = \alpha_{kl}^2 \int_a^b \Big(\sum_{i=-(k-l)}^{g} b_i^{(l)} B_i^{k+1-l}(x) \sum_{j=-(k-l)}^{g} b_j^{(l)} B_j^{k+1-l}(x) \Big) dx,$$

where $\alpha_{kl} = \prod_{j=1}^{l}(k+1-j)$. Further we can write $J_l(s_k)$ as a function of parameter $b = (b_{-k}, b_{-k+1}, \ldots, b_g)^T$

$$J_l(b) = \alpha_{kl}^2 \sum_{i=-(k-l)}^{g} \sum_{j=-(k-l)}^{g} b_i^{(l)} b_j^{(l)} \int_a^b B_i^{k+1}(x) B_j^{k+1}(x)dx = \alpha_{kl}^2 [b^{(l)}]^T M_{kl} b^{(l)},$$

where

$$M_{kl} := \begin{pmatrix} (B_{-k+l}^{k+1-l}, B_{-k+l}^{k+1-l}) & \ldots & (B_g^{k+1-l}, B_{-k+l}^{k+1-l}) \\ \vdots & & \vdots \\ (B_{-k+l}^{k+1-l}, B_g^{k+1-l}) & \ldots & (B_g^{k+1-l}, B_g^{k+1-l}) \end{pmatrix} \in \mathcal{M}_{g+k+1-l} \tag{14}$$

and

$$(B_i^{k+1-l}, B_j^{k+1-l}) := \int_a^b B_i^{k+1-l}(x) B_j^{k+1-l}(x)dx.$$

Matrix M_{kl} is p.d. because $B_i^{k+1-l} \geq 0$ and $B_{-g}^{k+1-l}, \ldots, B_g^{k+1-l}$ are basis functions (for more details see in [1], [3]). Using the relation (7) we get

$$J_l(b) = \alpha_{kl}^2 \, [S_l b]^T \, M_{kl} S_l b = \alpha_{kl}^2 ||b||_{N_{kl}}^2, \tag{15}$$

with matrices

$$N_{kl} := S_l^T M_{kl} S_l \in \mathcal{M}_{g+k+1}, \tag{16}$$

$$S_l = D_l L_l \ldots D_1 L_1 \in \mathcal{M}_{g+k+1-l,g+k+1},$$

$$D_j := diag\left(\frac{1}{\lambda_{i+k+1-j} - \lambda_i}\right)_{i=-(k-j),\ldots,g} \in \mathcal{M}_{g+k+1-j}$$

and bidiagonal matrix

$$L_j := \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix} \in \mathcal{M}_{g+k+1-j,g+k+2-j}.$$

Matrix N_{kl} is p.s.d. because with respect to the definition of matrix S_l, there is $rank(S_l) = g+k+1-l$ and thus $rank(N_{kl}) = g+k+1-l$. Let us remark that if we choose $l = 0$ then $S_0 = I$ and $N_{k0} = M_{k0}$ is p.d.

4.3 Unique solution of the optimal interpolatory problem

Owing to precedent two sections 4.1 and 4.2 we can rewrite our optimal interpolatory problem, which was described in section 1, as a following problem:

Problem *Our problem is to find a solution b^* of a consistent nonhomogenous equation*

$$C_{k+1}(x)b = y \tag{17}$$

for which

$$J_l(b) = \alpha_{kl}^2 ||b||_{N_{kl}}^2$$

is minimal.

In other words we wish to find a minimum N_{kl}-(semi)norm solution of (17). The corresponding technique was described in the section 3. Let us remind that $C_{k+1}(x) \in \mathcal{M}_{n,g+k+1}$ is the matrix with the rank$(C_{k+1}(x)) = n$ and the matrix $N_{kl} \in \mathcal{M}_{g+k+1}$ is p.d. for $l = 0$ and p.s.d. for $l \neq 0$. Let $Z \in \mathcal{M}_{g+k+1,g+k+1-n}$ be such a matrix that

$$C_{k+1}(x)Z = 0$$

and

$$\text{rank}([C_{k+1}^T(x), Z]) = g + k + 1,$$

then we can use for solving this problem the Theorem 3.9.

The important property of the matrix Z is that it has linearly independent columns $z_1, \ldots, z_{g+k+1-n}$ which are in the null space of $C_{k+1}(x)$, i.e.

$$z_i \in Ker(C_{k+1}(x)) := \{\delta : C_{k+1}(x)\delta = 0\}, \quad i = 1, \ldots, g + k + 1 - n$$

and therefore these vectors are basis vectors for the null space.

Owing to the Theorem 3.9. there is just one minimum N_{kl}-(semi)norm solution of (17) if and only if $Z^T N_{kl} Z$ is p.d.

If $l \neq 0$ then with respect to the relation (16) the matrix $N_{kl} \in \mathcal{M}_{g+k+1}$ with the rank$(N_{kl}) = g + k + 1 - l$ is p.s.d. Then it is easily verifed that the matrix $Z^T N_{kl} Z \in \mathcal{M}_{g+k+1-n}$ is p.d. if and only if $n \geq l$. If $l = 0$, the matrix $N_{k0} \in \mathcal{M}_{g+k+1}$ is p.d. and therefore $Z^T N_{k0} Z \in \mathcal{M}_{g+k+1-n}$ is p.d. The condition $n \geq l$ is fulfilled.

In such a way we have proved the following Theorem.

Theorem 4.1 *Let $C_{k+1}(x) \in \mathcal{M}_{n,g+k+1}$ be a matrix with* rank$(C_{k+1}(x)) = n$, *$Z \in \mathcal{M}_{g+k+1,g+k+1-n}$ be such a matrix that* rank$([C_{k+1}^T(x), Z]) = g + k + 1$, *$C_{k+1}(x)Z = 0$ and the matrix $N_{kl} \in \mathcal{M}_{g+k+1}$ be defined as in relation (16). Then there exists just one minimum N_{kl}-(semi)norm solution b^* of a consistent system (17) if and only if $n \geq l$. This solution is given as*

$$b^* = [C_{k+1}(x)]_{m(N_{kl})}^- y. \tag{18}$$

Now we can state the Theorem which describes necessary and sufficient condition under which there exists just one solution of our optimal interpolatory problem.

Theorem 4.2 *Let us have given sequence of knots $a < \lambda_1 < \ldots < \lambda_g < b$ and data (x_i, y_i), $a \leq x_i \leq b$, $i = 1, \ldots, n$. Then there exists just one spline $s_k(x)$ of degree $k > 0$, defined on interval $[a, b]$, with the given sequence of knots which interpolates data (x_i, y_i), $i = 1, \ldots, n$ and minimizes functional*

$$J_l(s_k) = \int_a^b \left[s_k^{(l)}\right]^2 dx, \quad l \in \{0, 1, \ldots, k-1\}$$

if and only if $l \leq n \leq g + k$ and there exists $\{\mu_1, \ldots, \mu_n\} \subset \{\lambda_{-k}, \ldots, \lambda_g\}$ with $\mu_i < \mu_{i+1}$, $i = 1, \ldots, n$ such that

$$\mu_i < x_i < \mu_{i+k+1}, \ i = 1, \ldots, n.$$

Proof Owing to the Theorem 2.2 and the section 4.1 we can see that the spline $s_k(x)$ of order $k > 0$ interpolating data (x_i, y_i), $i = 1, \ldots, n$ exists. The uniqueness follows from the Theorem 3.7 and the Theorem 4.1. □

Remark 4.3 If in the precedent Theorem the necessary and sufficient conditions hold then the optimal interpolatory spline has a unique representation

$$s_k(x) = \sum_{i=-k}^{g} b_i^* B_i^{k+1}(x), \tag{19}$$

with the B-spline coefficients $b^* = (b^*_{-k}, \ldots, b^*_g)^T$, which are given by the formula (18).

5 Calculation of the optimal interpolatory spline

In this section we describe an algorithm for computing spline $s_k(x)$ defined on interval $[a, b]$, with the given sequence of knots, interpolating given data and minimizing the functional (1).

Algorithm 5.1.

Input:
interval $[a, b]$
$k > 0$ degree of spline,
$l \in \{0, 1, \ldots, k-1\}$ degree of derivative in functional $J_l(s_k)$,
sequence of knots $a < \lambda_1 < \ldots < \lambda_g < b$
additional knots $\lambda_{-k} \leq \ldots \leq \lambda_0 = a$, $b = \lambda_{g+1} \leq \ldots \leq \lambda_{g+k+1}$
and data $x = (x_1, \ldots, x_n)^T$, $y = (y_1, \ldots, y_n)^T$
such that $a \leq x_i \leq b$, for $i = 1, \ldots, n$, $l \leq n \leq g + k$ and there exists
$\{\mu_1, \ldots, \mu_n\} \subset \{\lambda_{-k}, \ldots, \lambda_g\}$ with $\mu_i < \mu_{i+1}$, $i = 1, \ldots, n-1$ such that
$\mu_i < x_i < \mu_{i+k+1}$, $i = 1, \ldots, n$.

Steps:

1. Compute collocation matrix

$$C_{k+1}(x) = \begin{pmatrix} B_{-k}^{k+1}(x_1) & \dots & B_g^{k+1}(x_1) \\ \vdots & \ddots & \vdots \\ B_{-k}^{k+1}(x_n) & \dots & B_g^{k+1}(x_n) \end{pmatrix}.$$

   We can use MATLAB command *spcol* to compute this matrix.

2. For $i = -k+l, \dots, g$ and $j = -k+l, \dots, g$ calculate

$$\left(B_i^{k+1-l}, B_j^{k+1-l}\right) := \int_a^b B_i^{k+1-l}(x) B_j^{k+1-l}(x)dx.$$

   For computing these integrals we can use MATLAB commands *spmak, fncmb, fnint, fnval.*

3. Put $M_{kl} := \begin{pmatrix} \left(B_{-k+l}^{k+1-l}, B_{-k+l}^{k+1-l}\right) & \dots & \left(B_g^{k+1-l}, B_{-k+l}^{k+1-l}\right) \\ \vdots & & \vdots \\ \left(B_{-k+l}^{k+1-l}, B_g^{k+1-l}\right) & \dots & \left(B_g^{k+1-l}, B_g^{k+1-l}\right) \end{pmatrix}.$

4. If $l = 0$ then by using the Remark 3.4 and the Theorem 3.10 calculate $b^* = [C_{k+1}(x)]^-_{m(M_{kl})}\, y$, otherwise go on to the next steps.

5. For $i = 1, \dots, l$ compute

$$D_i := diag\left(\frac{1}{\lambda_{j+k+1-i} - \lambda_j}\right)_{j=-(k-i),\dots,g}$$

$$L_i := \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix} \in \mathcal{M}_{g+k+1-i,g+k+2-i}.$$

6. Put $S_l = D_l L_l \cdots D_1 L_1$.

7. Put $N_{kl} = S_l^T M_{kl} S_l$.

8. In view of the Remark 3.4 and the Theorem 3.10 compute

$$b^* = [C_{k+1}(x)]^-_{m(N_{kl})}\, y.$$

The unique optimal interpolatory spline $s_k(x)$ is given as

$$s_k(x) = \sum_{i=-k}^{g} b_i^* B_i^{k+1}(x), \tag{20}$$

with $b^* = (b_{-k}^*, \dots, b_g^*)^T$.

Example 5.1 For $\mathbf{x} = -1 : 2 : 11$, values of the function $y = (5 - x)\cos(x)$ and $\mathbf{knots} = \mathbf{x}$ we have computed the natural cubic interpolatory spline and the cubic interpolatory splines which minimize functional $J_l(s_3)$ for $l = 0, 1, 2$. These splines are plotted on Fig. 1. The natural cubic interpolatory spline and the optimal interpolatory spline which minimizes $J_2(s_3)$ are identical (solid line). The optimal interpolatory spline for $l = 1$ is plotted by dashed line and for $l = 0$ by dash-dotted line. The minimal values of the functional are $J_2 = 326.09$, $J_1 = 112.5$, $J_0 = 31.38$.

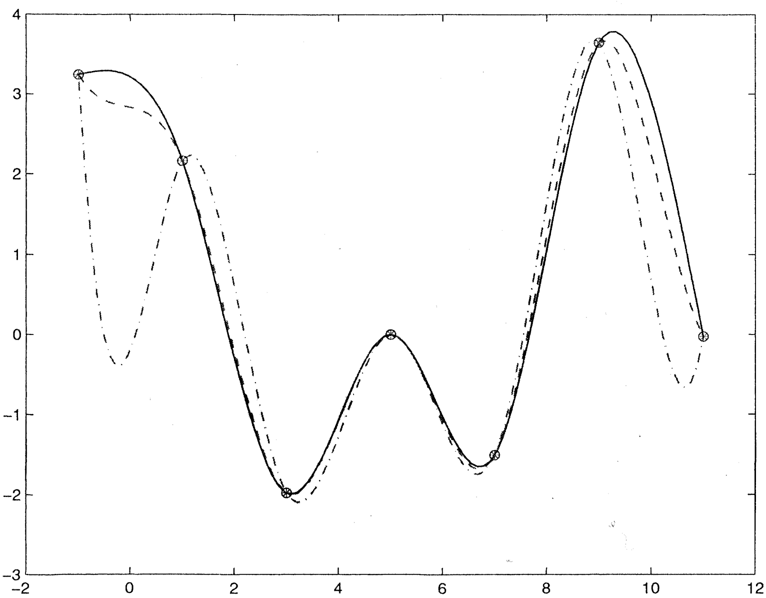

Fig.1

Example 5.2 Let us have given $\mathbf{x} = -1 : 2 : 11$, values $y = (5 - x)\cos(x)$ and $\mathbf{knots} = [-1, 0 : 2 : 10, 11]$. There are plotted the function $f(x) = (5 - x)\cos(x)$ (solid line), the natural cubic interpolatory spline with knots in x_i (dashed line) and the cubic interpolatory spline with given sequence of **knots** which minimizes $J_2(s_3)$ (dash-dotted line) on Fig. 2. The minimal values of the functional are 326.09 for the natural cubic interpolatory spline and 864.71 for the optimal cubic interpolatory spline. We can see that the value of functional for the optimal cubic interpolatory spline is greater than for the natural cubic interpolatory spline, but this spline approximates given function better than the other.

Example 5.3 On Fig. 3 we can see optimal splines of degree $k = 1, 2, 3$ with $\mathbf{knots} = -2 : 2 : 12$ which interpolate given data $\mathbf{x} = -1 : 2 : 11$, $y = (5 - x)\cos(x)$ and minimize the functional $J_0(s_k)$. The minimal values of functional are $J_0(s_1) = 213.35$, $J_0(s_2) = 56.82$ and $J_0(s_3) = 87.54$.

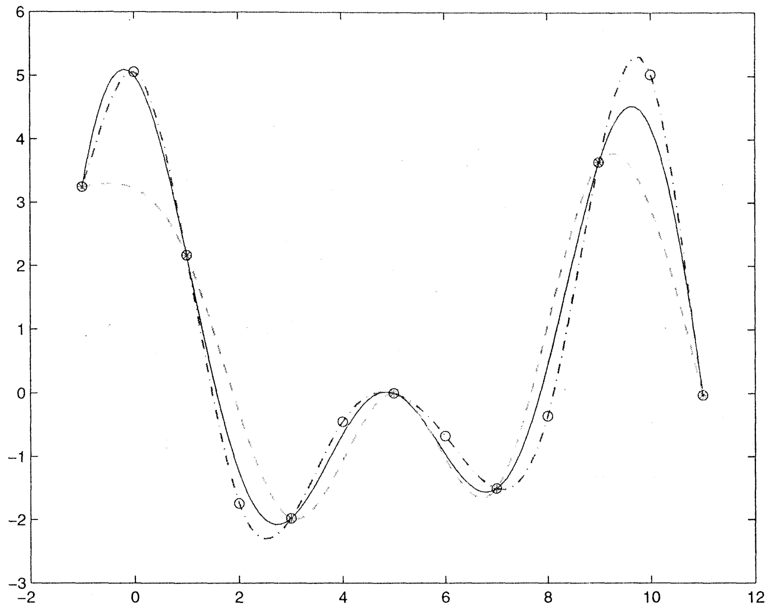
6
5
4
3
2
1
0
−1
−2
−3
−2
0
2
4
6
8
10
12

Fig. 2

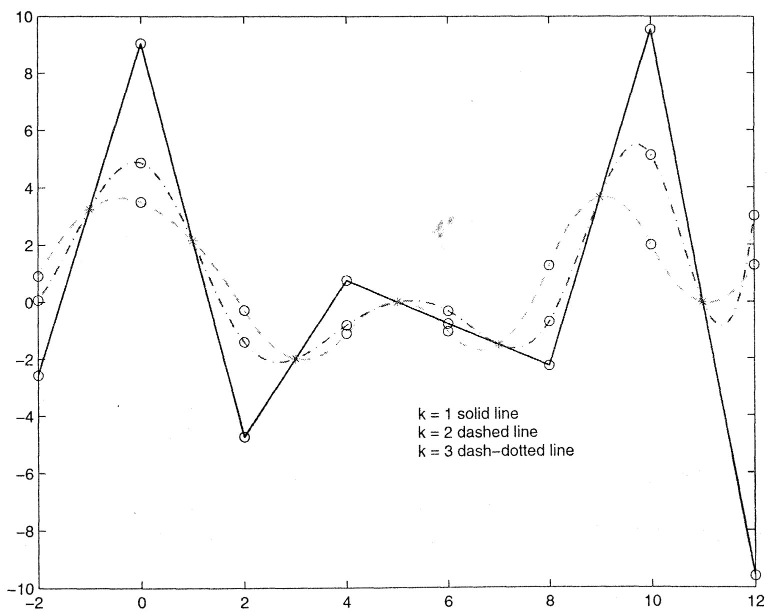
10
8
6
4
2
0
−2
−4
−6
−8
−10
−2
0
2
4
6
8
10
12
k = 1 solid line
k = 2 dashed line
k = 3 dash−dotted line

Fig. 3

6 Conclusion

We know that if there are given data (x_i, y_i), $a \leq x_i \leq b$, $i = 1, \ldots, n$ then there exists unique cubic spline with knots x_i which interpolates data (x_i, y_i), satiesfies natural conditions (i.e. zero second derivative at points a and b) and which minimizes functional $J_2(s_3)$ on the class of function $W_2^2(a, b)$. This spline is called the natural cubic interpolatory spline. Similar variational properties were generalized for spline of odd degree and latter too for spline of even degree. More information we can find for example in [1], [6].

In practise we need not know all values y_i in knots x_i or some values may not be exact so that there is no sence to require their interpolation. Under certain conditions, which are described in the Theorem 4.2, we can separate knots and interpolatory points. That way we have free parameters, which we can use to the minimization of the functional $J_l(s_k)$. If we consider only the class of splines of degree $k > 0$ with the given sequence of knots, we can solve this problem as the problem of optimal interpolation, which is described in this paper.

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