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L-SPLINE INTERPOLATION FOR DIFFERENTIAL OPERATORS OF ORDER 4 WITH CONSTANT COEFFICIENTS

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Abstract

In this paper it is shown that many features from polynomial spline methods used in nonparametric regression and smoothing procedures carry over to the class of L-splines where L is a linear differential operator of order 4 with constant coefficients. Special attention is given to the question whether an analogue of the Reinsch algorithm is valid and criteria are given such that the associated matrix R is strictly diagonal dominant.
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1. Introduction. Spline interpolation and smoothing provide an important technique in nonparametric methods for data analysis, [1–4]. As outlined in [5] the extension of cubic spline smoothing to the setting of L-splines allows to include additional prior knowledge for estimating the data and to retain several aspects of the data. For example, for the estimation of the gross domestic product data it is assumed that the model curve is a linear combination of the functions

$$1, \exp(\gamma t), \sin \omega t, \cos \omega t, \tag{1}$$

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while for melanoma data the model curve is linear combination of

$$1, t, \sin \omega t, \cos \omega t. \tag{2}$$

In both examples the model curve is a solution of a linear differential operator L with constant coefficients of order $N+1$, given by

$$L = L_{(\lambda_0,\ldots,\lambda_N)} = \prod_{j=0}^{N} \left(\frac{d}{dx} - \lambda_j \right), \tag{3}$$

where $\lambda_0, \ldots, \lambda_N$ are complex numbers. Let us recall that a function $g : [a,b] \to \mathbb{C}$ is an L-spline of order $N+1$ with knots $t_1 < \cdots < t_n$ if g is $N-1$ times continuously differentiable such that the restriction of g to each interval $[t_j, t_{j+1}]$ is a solution of the equation $L_N(g) = 0$.

Let us note that special classes of L-splines are an important component of the theory of polysplines and its applications, cf. [6–11].

In many textbooks, like [12,13] an efficient algorithm for L-spline smoothing is described in detail and usually it is based on reproduction kernel techniques associated to the differential operator. In this paper we want to describe an algorithm for linear differential operators L of order 4 which mimics the orginal algorithm of Reinsch from 1967 as closely as possible, [14]. An important feature of this algorithm is the fact that for given real numbers $t_1 < \cdots < t_n$ with $n > 2$ there exists a symmetric positive definite $(n-2) \times (n-2)$ matrix R and a $n \times (n-2)$ matrix Q and such that

$$Q^T \mathbf{g} = R\gamma \tag{4}$$

for any natural cubic spline g with knots $t_1 < \cdots < t_n$, where

$$\mathbf{g}^T = (g(t_1), g(t_2), \ldots, g(t_n)) \tag{5}$$

$$\gamma^T = \left(g''(t_2), g''(t_3), \ldots, g''(t_{n-1}) \right). \tag{6}$$

The matrix R can be described explicitly: it has tridiagonal form and for the diagonal and off-diagonal we have

$$R_{jj} = \frac{1}{3}(h_{j-1} + h_j) \text{ and } R_{j,j+1} = R_{j+1,j} = \frac{1}{6} h_j,$$

where $h_j = t_{j+1} - t_j$. Moreover a simple algorithm allows to compute the interpolating natural spline in $O(n)$ arithmetic operations.

Given a general linear differential operator $L_{(\lambda_0,\ldots,\lambda_3)}$ with constant coefficients of order 4 we define a $(n-2) \times (n-2)$ matrix R and a $n \times (n-2)$ matrix Q such that the relation

$$Q^T \mathbf{g} = R\gamma$$

holds for the vectors $\mathbf{g}$ and γ, defined by

$$\mathbf{g}^T = \left(g\left(t_1\right), g\left(t_2\right), \ldots, g\left(t_n\right)\right) \tag{7}$$

$$\gamma^T = \left(L_{(\lambda_0,\lambda_1)} g\left(t_2\right), L_{(\lambda_0,\lambda_1)} g\left(t_3\right), \ldots, L_{(\lambda_0,\lambda_1)} g\left(t_{n-1}\right)\right). \tag{8}$$

The matrix R is tridiagonal and a simple algorithm allows to compute the interpolating natural spline in O(n) arithmetic operations. To facilitate the exposition we follow the notations given in [13].

The matrices R and Q depend on the differential operator given by the values $\lambda_0, \lambda_1, \lambda_2, \lambda_3$. In order to describe the matrices we need the notion of the *fundamental function* Φ_{Λ_N} with respect to the vector $\Lambda_N = (\lambda_0, \ldots, \lambda_N)$: there exists a unique solution Φ_{Λ_n} of the equation $L_N u = 0$ such that $\Phi_{\Lambda_N}(0) = \cdots = \Phi_{\Lambda_N}^{(N-1)}(0) = 0$ and $\Phi_{\Lambda_N}^{(N)}(0) = 1$, see [6,15]. In Section 2 we shall recall several properties of the fundamental function Φ_{Λ_N} and describe its relationship with the Green function. In Section 3 we will show that the matrix R is tridiagonal and that the diagonal and off-diagonal entries are given by

$$R_{j,j} = \rho\left(t_j - t_{j-1}\right) - \rho\left(-\left(t_{j+1} - t_j\right)\right) \tag{9}$$

$$R_{j,j+1} = \sigma\left(t_{j+1} - t_j\right) \text{ and } R_{j+1,j} = -\sigma\left(-\left(t_{j+1} - t_j\right)\right), \tag{10}$$

where ρ and σ are functions defined by

$$\rho(x) = \frac{\Phi'_{(\lambda_0,\ldots,\lambda_3)}(x)\,\Phi_{(\lambda_0,\lambda_1)}(x) - \Phi_{(\lambda_0,\ldots,\lambda_3)}(x)\,\Phi'_{(\lambda_0,\lambda_1)}(x)}{\Phi_{(\lambda_0,\lambda_1)}(x)\,\Phi_{(\lambda_2,\lambda_3)}(x)}, \tag{11}$$

$$\sigma(x) = \frac{\Phi_{(\lambda_0,\ldots,\lambda_3)}(x)}{\Phi_{(\lambda_0,\lambda_1)}(x)\,\Phi_{(\lambda_2,\lambda_3)}(x)}. \tag{12}$$

In a similar way the matrix Q is defined. In Section 4 we will show that the entries in (9) and (10) are positive provided that $\lambda_0, \ldots, \lambda_3$ are real. We provide in Section 5 a simple sufficient criterion such that the matrix R is strictly diagonal dominant. In the case that (λ_0, λ_1) and (λ_2, λ_3) are conjugation invariant we show that for any $\varepsilon > 0$ there exists $\delta > 0$ such that the estimate

$$|R_{j,j-1}| + |R_{j,j+1}| \leq \left(\frac{1}{2} + \varepsilon\right)|R_{jj}|$$

holds for all $t_1 < \cdots < t_n$ such that $t_{j+1} - t_j \leq \delta$ for $j = 1, \ldots, n-1$. For the example in (2) we shall provide exact estimates. We show that for the special set $\Lambda_3 = (a, -a, -b, b) \in \mathbb{R}^4$ with $0 \leq a \leq b$ the estimate

$$R_{j,j-1} + R_{j,j+1} \leq \frac{1}{2} R_{jj}$$

holds. This estimate is important for the study and applications of polysplines (see [7–11,16]) which requires a deep analysis of L-splines.

The present paper generalizes the results obtained in [17] for special classes of L-splines, see also [18].

The detailed proofs will appear elsewhere.

2. The fundamental function. We assume that we are given a vector $\Lambda \in \mathbb{C}^{N+1}$, with the first coordinate having index 0, namely

$$\Lambda_N = (\lambda_0, \ldots, \lambda_N) .$$

For the differential operator L_N defined in (3) we introduce the solution set:

$$E(\lambda_0, \ldots, \lambda_N) := \left\{ f \in C^N(\mathbb{R}, \mathbb{C}) : L_N f = 0 \right\},$$

where $C^N(\mathbb{R}, \mathbb{C})$ is the space of all N-times continuously differentiable complex-valued functions $f : \mathbb{R} \to \mathbb{C}$. The elements in $E_{(\lambda_0,\ldots,\lambda_N)}$ are called *exponential polynomials* or *L-polynomials,* and $\lambda_0, \ldots, \lambda_N$ are called *exponents* or *frequencies* (see e.g. Chapter 3 in [19]).

We say that the space $E_{(\lambda_0,\ldots,\lambda_N)}$ is *closed under complex conjugation*, if for $f \in E_{(\lambda_0,\ldots,\lambda_N)}$ the complex conjugate function $\overline{f}$ is again in $E_{(\lambda_0,\ldots,\lambda_N)}$. It is easy to see that for complex numbers $\lambda_0, \ldots, \lambda_N$ the space $E_{(\lambda_0,\ldots,\lambda_N)}$ is closed under complex conjugation if and only if there exists a permutation σ of the indices $\{0, \ldots, N\}$ such that $\overline{\lambda_j} = \lambda_{\sigma(j)}$ for $j = 0, \ldots, N$. In other words, $E_{(\lambda_0,\ldots,\lambda_N)}$ is closed under complex conjugation if and only if the vector $\Lambda_N = (\lambda_0, \ldots, \lambda_N)$ is equal up to reordering to the conjugate vector $\overline{\Lambda_N}$. In this case we say that Λ_N is *conjugation invariant.*

It is well known that for $\Lambda_N = (\lambda_0, \ldots, \lambda_N) \in \mathbb{C}^{N+1}$ there exists a unique solution $\Phi_{\Lambda_N} \in E_{(\lambda_0,\ldots,\lambda_N)}$ to the Cauchy problem

$$\Phi_{\Lambda_N}(0) = \ldots = \Phi_{\Lambda_N}^{(N-1)}(0) = 0 \text{ and } \Phi_{\Lambda_N}^{(N)}(0) = 1.$$

We shall call Φ_{Λ_N} the *fundamental function* in $E_{(\lambda_0,\ldots,\lambda_N)}$ (see e.g. [6,15]). An explicit formula for Φ_{Λ_N} is

$$\Phi_{\Lambda_N}(x) = \frac{1}{2\pi i} \int_{\Gamma_r} \frac{e^{xz}}{(z-\lambda_0)\cdots(z-\lambda_N)} dz, \tag{13}$$

where Γ_r is the path in the complex plane defined by $\Gamma_r(t) = re^{it}$, $t \in [0, 2\pi]$, surrounding all the complex numbers $\lambda_0, \ldots, \lambda_N$. In particular, for $N = 0$ we have

$$\Phi_{(\lambda_0)}(x) = e^{\lambda_0 x}.$$

Note that (13) implies the useful formula

$$\left(\frac{d}{dx} - \lambda_{N+1} \right) \Phi_{(\lambda_0,\ldots,\lambda_{N+1})}(x) = \Phi_{(\lambda_0,\ldots,\lambda_N)}(x) . \tag{14}$$

If $\Lambda_N = \overline{\Lambda_N}$, then we see that the conjugate of Φ_{Λ_N} is again in $E_{(\lambda_0,\ldots,\lambda_N)}$, and by uniquessness of the fundamental function we conclude:

Proposition 1. *If $\Lambda_N = \overline{\Lambda_N}$, then $\Phi_{\Lambda_N}(t)$ is a real-valued function.*

Proposition 2. *If $\lambda_0, \dots, \lambda_N$ are real numbers, then $\Phi_{(\lambda_0,\dots,\lambda_N)}(t) > 0$ for all $t > 0$.*

Proposition 2 is based on the fact that $\Phi_{(\lambda_0,\dots,\lambda_N)}(\cdot)$ has at most N zeros (including multiplicities) and all of them are concentrated at $t = 0$.

We may prove directly the following:

Proposition 3. *Let λ_0, λ_1 be complex numbers. Then*

$$\Phi_{(\lambda_0,\lambda_1)}(-x)\,\Phi_{(\lambda_2,\lambda_3)}(-x) = e^{-(\lambda_0+\lambda_1+\lambda_2+\lambda_3)x}\Phi_{(\lambda_0,\lambda_1)}(x)\,\Phi_{(\lambda_2,\lambda_3)}(x). \tag{15}$$

The function $\Phi_{(\lambda_0,\lambda_1)}(x)\,\Phi_{(\lambda_2,\lambda_3)}(x)$ is even if and only if $\lambda_0 + \dots + \lambda_3 = 0$.

3. Computation of the matrix $\boldsymbol{R}$. We assume that $t_1 < \dots < t_n$ are real numbers such that

$$\Phi_{(\lambda_0,\lambda_1)}(t_{j+1} - t_j) \neq 0 \quad \text{and} \quad \Phi_{(\lambda_2,\lambda_3)}(t_{j+1} - t_j) \neq 0 \tag{16}$$

for $j = 1, \dots, n-1$. In the general case condition (16) holds if $t_j - t_j$ is sufficiently small for $j = 1, \dots, n-1$. For complex numbers $\lambda_0, \dots, \lambda_3$ we define the linear differential operators

$$L_1 = \left(\frac{d}{dt} - \lambda_0\right)\left(\frac{d}{dt} - \lambda_1\right) \text{ and } L_2 = \left(\frac{d}{dt} - \lambda_2\right)\left(\frac{d}{dt} - \lambda_3\right).$$

The following is the main result of this section:

Theorem 4. *Let $\lambda_0, \dots, \lambda_3$ be complex numbers and $t_1 < \dots < t_n$ such that (16) holds, and let g be a natural spline for $\Lambda_3 = (\lambda_0, \lambda_1, \lambda_2, \lambda_3)$ with interpolation data $g_1, \dots, g_n$. Then there exist a $n\times(n-2)$ matrix Q and a symmetric $(n-2)\times(n-2)$ matrix R such that*

$$Q^T\mathbf{g} = R\gamma. \tag{17}$$

Theorem 5. *Let $\lambda_0, \dots, \lambda_3$ be complex numbers and $t_1 < \dots < t_n$ such that (16) holds, and let g be a natural spline for the operator L_1L_2 with interpolation data $g_1, \dots, g_n$. Then the tridiagonal matrix R is given by*

$$R_{j,j} = \rho(t_j - t_{j-1}) - \rho(-(t_{j+1} - t_j))$$
$$R_{j,j+1} = \sigma(t_{j+1} - t_j) \text{ and } R_{j+1,j} = -\sigma(-(t_{j+1} - t_j))$$

and ρ and σ are defined in (11) and (12).

In the same manner one proves the following result:

Theorem 6. *The $n \times (n-2)$ matrix Q is given for $i = 1, \dots, n$ and $j = 2, 3, \dots, n-1$, by*

$$q_{j-1,j} = -\frac{\Phi'_{(\lambda_0,\lambda_1)}(t - t_j)}{\Phi_{(\lambda_0,\lambda_1)}(t_{j-1} - t_j)}, \qquad q_{j+1,j} = \frac{\Phi'_{(\lambda_0,\lambda_1)}(t - t_j)}{\Phi_{(\lambda_0,\lambda_1)}(t_{j+1} - t_j)} \tag{18}$$

and

$$q_{jj} = \frac{\Phi'_{(\lambda_0,\lambda_1)}(t - t_{j+1})}{\Phi_{(\lambda_0,\lambda_1)}(t_j - t_{j+1})} - \frac{\Phi'_{(\lambda_0,\lambda_1)}(t - t_{j-1})}{\Phi_{(\lambda_0,\lambda_1)}(t_j - t_{j-1})}.$$

4. Positivity of the entries of the matrix R. In the following we want to analyze under which conditions the entries of the matrix R are real or even positive. If the vector $\Lambda_N = (\lambda_0, \ldots, \lambda_N)$ is conjugation invariant, the fundamental function Φ_{Λ_N} is real-valued. If (λ_0, λ_1) and (λ_2, λ_3) are conjugation invariant, then $(\lambda_0, \lambda_1, \lambda_2, \lambda_3)$ is conjuation invariant and we infer that

$$\Phi_{(\lambda_0,\lambda_1)}, \Phi_{(\lambda_2,\lambda_3)}, \Phi_{(\lambda_0,\lambda_1,\lambda_2,\lambda_3)} \text{ and } \Phi'_{(\lambda_0,\lambda_1,\lambda_2,\lambda_3)}$$

are real-valued functions. Hence under the additional assumption that

$$\Phi_{(\lambda_0,\lambda_1)}(t) \neq 0 \text{ and } \Phi_{(\lambda_2,\lambda_3)}(t) \neq 0 \text{ for } t \in (0, \delta)$$

for some $\delta > 0$, the functions $\rho(x)$ and $\sigma(x)$ are real-valued and well-defined and all entries of the matrices R and Q are real-valued for all $t_1 < \cdots < t_n$ such that $|t_{j+1} - t_j| < \delta$ for $j = 1, \ldots, n-1$.

Corollary 7. *Suppose that $\lambda_0, \ldots, \lambda_3$ are real numbers. Then $R_{j,j}$ and $R_{j,j+1}$ and $R_{j-1,j}$ are positive numbers for all $t_1 < \cdots < t_n$.*

5. Diagonal dominance of the matrix R. The notion of diagonal dominance of matrices is very important in numerical analysis, cf. [20]. We start with the following general criterion:

Theorem 8. *Assume that $\rho(x)$ and $-\rho(-x)$ are positive on the interval $(0, \delta)$, and let $M_\delta > 0$ be such that*

$$|\sigma(x)| \leq M_\delta |\rho(-x)| \text{ for all } x \in [-\delta, \delta]. \tag{19}$$

Then the estimate

$$|R_{j,j-1}| + |R_{j,j+1}| \leq M_\delta |R_{j,j}|$$

holds for all partitions $t_1 < \cdots < t_n$ such that $t_{j+1} - t_j \leq \delta$ for $j = 1, \ldots, n$.

We illustrate the result by two examples:

Proposition 9. *If $\Lambda_3 = (0, 0, -b, b)$ for some real $b \neq 0$, then $R_{j,j-1} + R_{j,j+1} \leq \frac{1}{2} R_{j,j}$ for all $t_1 < \cdots < t_n$.*

If we allow complex frequencies, we obtain a weaker result:

Theorem 10. *Let $0 < \delta < \pi$. Then for $\Lambda_3 = (0, 0, -i\beta, i\beta)$ with real $\beta > 0$ we have*

$$R_{j,j-1} + R_{j,j+1} \leq \frac{\sin\delta - \delta}{\delta\cos\delta - \sin\delta} R_{j,j} < R_{j,j}$$

for all $t_1 < \cdots < t_n$ such that $\beta(t_{j+1} - t_j) \leq \delta$ for $j = 1, \ldots, n-1$.

Theorem 11. *Suppose that (λ_0, λ_1) and (λ_2, λ_3) are conjugation invariant and $\varepsilon > 0$. Then there exists $\delta > 0$ such that the estimate*

$$|R_{j,j-1}| + |R_{j,j+1}| \leq \left(\frac{1}{2} + \varepsilon\right) |R_{j,j}|$$

holds for all partitions $t_1 < \cdots < t_n$ such that $t_{j+1} - t_j \leq \delta$ for $j = 1, \ldots, n$.

We call the set Λ_N *symmetric* if there exists a permutation π of the set $\{0, \dots, N\}$ such that $-\lambda_j = \lambda_{\pi(j)}$ for $j = 0, \dots, N$, or, symbolically, $-\Lambda_N = \Lambda_N$. If Λ_N is symmetric, then

$$\Phi_{\Lambda_N}(-x) = (-1)^N \, \Phi_{\Lambda_N}(x) .$$

This formula shows that for odd N the complex-valued function Φ_{Λ_N} is odd, and for even N the function Φ_{Λ_N} is even.

One may prove the following main result concerning symmetric sets Λ_N.

Theorem 12. *The matrix R for $\Lambda_3 = (\lambda_0, \dots, \lambda_3)$ is symmetric for any choice of interpolation points $t_1 < \dots < t_n$ if and only if Λ_3 is symmetric.*

For a special class of examples which occur naturally in the study of polysplines on parallel strips (cf. [6]), we obtain an explicit estimate.

Theorem 13. *Let $0 < a < b$ and $\Lambda_3 = (a, -a, -b, b)$. Then the following estimate holds*

$$R_{j,j-1} + R_{j,j+1} \leq \frac{1}{2} R_{j,j} .$$

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