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On the Construction of Optimal Monotone Cubic Spline Interpolations*

Sigrid Fredenhagen, Hans Joachim Oberle, and Gerhard Opfer

Institute of Applied Mathematics, University of Hamburg, Bundesstrasse 55, D-20146 Hamburg, Germany

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In this paper we derive necessary optimality conditions for an interpolating spline function which minimizes the Holladay approximation of the energy functional and which stays monotone if the given interpolation data are monotone. To this end optimal control theory for state-restricted optimal control problems is applied. The necessary conditions yield a complete characterization of the optimal spline. In the case of two or three interpolation knots, which we call the *local* case, the optimality conditions are treated analytically. They reduce to polynomial equations which can very easily be solved numerically. These results are used for the construction of a numerical algorithm for the optimal monotone spline in the general (global) case via Newton's method. Here, the local optimal spline serves as a favourable initial estimation for the additional grid points of the optimal spline. Some numerical examples are presented which are constructed by FORTRAN and MATLAB programs. © 1999 Academic Press

1. INTRODUCTION

In recent years the problem of shape-preserving interpolation and approximation has become a wide field of interest. For a given grid $I_0 = \{t_1, ..., t_n\}$, where

$$a = t_1 < t_2 < \cdots < t_n = b, \tag{1.1}$$

and given interpolation values x_j, $j = 1, ..., n$, where $n > 2$, one seeks a function x, which interpolates the given data (t_j, x_j), which has certain smoothness properties and which preserves certain properties of the given values like non-negativity, monotonicity, or convexity. The different

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methods for the construction of such interpolation functions are characterized by different demands with respect to the degree of smoothness and by local or global constructions, see, for example, Akima [1], Fritsch and Carlson [8], and Schmidt and Hess [19].

The authors considered in several investigations also some kind of optimality conditions generalizing the Holladay property of the classical cubic spline, cf. Hornung [10, 11], Oberle and Opfer [15, 17], Fischer *et al.* [7], Dontchev [6], or Andersson and Elfving [2]. We consider in this paper in continuation of these investigations the problem of optimal monotone spline interpolation from a local and global point of view.

Problem 1.1. Given the grid (1.1) and numbers x_j, $j=1, 2, ..., n$, we seek a minimizer x of the Holladay functional

$$J(x) := \tfrac{1}{2} \int_a^b (x''(t))^2 \, dt \tag{1.2}$$

subject to the constraints

$$x(t_j) = x_j, \qquad j = 1, ..., n, \tag{1.3}$$

$$x'(t) \geqslant x'_{\min}, \tag{1.4}$$

where $x'_{\min}$ is a given number, and it is assumed that the following property holds for the given interpolation data:

$$(x_{j+1} - x_j) > x'_{\min} \cdot (t_{j+1} - t_j), \qquad j = 1, ..., n-1. \tag{1.5}$$

If s is the linear spline connecting the given data points, the condition (1.5) means that $s'(t) > x'_{\min}$ for all $t \in [t_1, t_n] \backslash I_0$.

In general, it is demanded that x belongs to the Sobolev space $W_2^2[a, b]$ of all functions with absolutely continuous first derivative and square integrable second derivative. But not much is lost if the problem is restricted to functions $x \in C_s^2[a, b]$, which are continuously differentiable and have a piecewise continuous second derivative.

There are some obvious modifications of Problem 1.1 which can be treated in the same way and which are relevant in a certain context.

Problem 1.2. This is the same as Problem 1.1 with additional boundary conditions for the first derivative,

$$x'(a) = b_1, \qquad x'(b) = b_n, \tag{1.6}$$

where b_1, b_n are given numbers with $b_1, b_n > x'_{\min}$.

Problem 1.3. This is the same as Problem 1.1 or Problem 1.2; however, the slope is bounded also from above:

$$x'_{\min} \leqslant x'(t) \leqslant x'_{\max}, \qquad t \in [a, b]. \tag{1.7}$$

A solution to Problem 1.1 is usually called a *natural* spline.

2. NECESSARY CONDITIONS DERIVED BY OPTIMAL CONTROL THEORY

We want to apply the necessary conditions of optimal control theory to Problem 1.1. Therefore, we consider a general optimal control problem with an inequality constraint put on the state variables. This control problem has the following form:

Problem 2.1. Determine a piecewise continuous *control variable* $u(t) \in \mathbb{R}$, $a \leqslant t \leqslant b$, which minimizes the functional

$$J(u) := \int_a^b f_0(y(t), u(t))\, dt \tag{2.1}$$

subject to the constraints

$$y'(t) = f(y(t), u(t)), \qquad a \leqslant t \leqslant b, \qquad \text{(a.e.)}, \tag{2.2}$$

$$r(y(t_1), y(t_2), ..., y(t_n)) = 0, \tag{2.3}$$

$$g(y(t)) \leqslant 0. \tag{2.4}$$

The vector $y(t) \in \mathbb{R}^m$ denotes the *state variables*. The functions f_0: $\mathbb{R}^{m+1} \to \mathbb{R}$, f: $\mathbb{R}^{m+1} \to \mathbb{R}^m$, r: $\mathbb{R}^{n \cdot m} \to \mathbb{R}^k$, and g: $\mathbb{R}^m \to \mathbb{R}$ are assumed to be sufficiently smooth. Equation (2.2) describes the *state equations*, Eq. (2.3) the *multipoint-boundary conditions*, and Eq. (2.4) the *state variable inequality constraint*.

We summarize the necessary conditions due to Jacobson *et al.* [12] and Maurer [14]. Let (y^*, u^*) denote a solution of the general optimal control Problem 2.1. It is assumed that the *solution structure* consists of a finite number of *contact points*, *boundary subarcs*, and *free subarcs*. Here, a boundary subarc is an interval $I = [\tau_1, \tau_2]$, $\tau_1 < \tau_2$, of maximal length such that $g[t] := g(y^*(t))$ vanishes identically on I, τ_1 is called the *entry point*, and τ_2 the *exit point* of the boundary subarc I. An interval $I = [\tau_1, \tau_2]$ is called a *free subarc*, if $g[t] < 0$, $\tau_1 < t < \tau_2$, holds and, finally, a point τ is called a *contact point*, if it is an isolated zero of $g[t]$. Entry, exit, or contact points are summarized as *junction points*.

Now, the necessary conditions can be stated as follows. There exist piecewise continuously differentiable *adjoint variables* $\lambda(t) \in \mathbb{R}^m$, $\eta(t) \geqslant 0$, and parameters $\lambda_0 \geqslant 0$, $l \in \mathbb{R}^k$, $\alpha_j \geqslant 0$, $j=1, ..., n$, $\mu(\tau) \geqslant 0$, where τ represents an arbitrary junction point, such that

$$(\lambda_0, \lambda(t), \eta(t), l_1, ..., l_k, \alpha_1, ..., \alpha_n, \mu(\tau_1), \mu(\tau_2), ...) \not\equiv 0 \tag{2.5}$$

for $t \in [a, b]$ and that for the augmented Hamiltonian (Lagrangian)

$$H(y, u, \lambda, \eta, \lambda_0) := \lambda_0 f_0(y, u) + \lambda^T f(y, u) + \eta g(y) \tag{2.6}$$

the following properties hold:

(1) *Adjoint differential equations,*

$$\lambda'(t) = -H_y(y(t), u(t), \lambda(t), \eta(t), \lambda_0). \tag{2.7}$$

(2) *Minimum principle,*

$$u^*(t) = \arg\min_u H(y^*(t), u, \lambda(t), \eta(t), \lambda_0). \tag{2.8}$$

(3) *Natural boundary conditions,*

$$\begin{aligned} \lambda(t_1) &= -\frac{\partial}{\partial y(t_1)} (l^{\mathrm{T}} r(y(t_1), ..., y(t_n)) + \alpha_1 g(y(t_1))), \\ \lambda(t_j^+) - \lambda(t_j^-) &= -\frac{\partial}{\partial y(t_j)} (l^{\mathrm{T}} r(y(t_1), ..., y(t_n)) + \alpha_j g(y(t_j))), \\ & \qquad j = 2, ..., n-1, \\ \lambda(t_n) &= \frac{\partial}{\partial y(t_n)} (l^{\mathrm{T}} r(y(t_1), ..., y(t_n)) + \alpha_n g(y(t_n))). \end{aligned} \tag{2.9}$$

(4) *Complementarity condition,*

$$\begin{aligned} \eta(t) \cdot g[t] &= 0, \qquad a \leqslant t \leqslant b, \\ \alpha_j \cdot g[t_j] &= 0, \qquad j = 1, ..., n. \end{aligned} \tag{2.10}$$

(5) *Jump conditions (τ junction point),*

$$\begin{aligned} \lambda(\tau^+) - \lambda(\tau^-) &= -\mu(\tau)\, g_y(y(\tau)), \\ H[\tau^+] - H[\tau^-] &= 0. \end{aligned} \tag{2.11}$$

Here, the abbreviation $H[t] := H(y^*(t), u^*(t), \lambda(t), \eta(t), \lambda_0)$ is used.

Note, that, in extension of the general formulation (cf. Opfer and Oberle [17]), the α_j-terms occur in Eqs. (2.9), see Chudej [4]. This is because in our application the fixed knots t_j may be located within a boundary subarc of the constraint g.

In order to apply the necessary conditions to Problem 1.1, we substitute $y_1(t) := x(t)$, $y_2(t) := x'(t)$, and $u(t) := x''(t)$. Then, Problem 1.1 takes the form of the general optimal control Problem 2.1 with $f_0 := u^2/2$, $f := (y_2, u)^T$, $r_j := y_1(t_j) - x_j$, $j = 1, ..., n$, and $g(y) := x'_{\min} - y_2$. With these relations the augmented Hamiltonian takes the form

$$H = \tfrac{1}{2}u^2\lambda_0 + \lambda_1 y_2 + \lambda_2 u + \eta(x'_{\min} - y_2). \tag{2.12}$$

The adjoint differential equations are

$$\lambda_1'(t) = 0, \qquad \lambda_2'(t) = \eta - \lambda_1, \tag{2.13}$$

and the natural boundary conditions and the jump relations can be written as

$$\begin{aligned}
&\lambda_1(t_1) = -l_1, && \lambda_2(t_1) = \alpha_1,\\
&\lambda_1(t_j^+) = \lambda_1(t_j^-) - l_j, && \lambda_2(t_j^+) = \lambda_2(t_j^-) + \alpha_j,\ 2 \leqslant j \leqslant n-1,\\
&\lambda_1(t_n) = l_n, && \lambda_2(t_n) = -\alpha_n,\\
&\lambda_1(\tau^+) = \lambda_1(\tau^-), && \lambda_2(\tau^+) = \lambda_2(\tau^-) + \mu(\tau),\\
&H[\tau^+] = H[\tau^-].
\end{aligned} \tag{2.14}$$

The degenerate case $\lambda_0 = 0$ can be excluded by an explicit argument: By the minimum principle the assumption $\lambda_0 = 0$ yields $\lambda_2 \equiv 0$ on the whole interval $[a, b]$. Therefore, from Eq. (2.13), it follows that λ_1 vanishes on free subarcs.

On the other hand, Eqs. (2.13)–(2.14) show that λ_1 is a piecewise constant function and jumps of λ_1 can occur only at the given interpolation knots. Now, the assumption (1.5) ensures that each interpolation interval $[t_j, t_{j+1}]$ contains some points of a free subarc. Therefore, λ_1 also vanishes identically on the whole interval $[a, b]$, and so all adjoint variables do. Altogether, the degeneration assumption contradicts the necessary condition (2.5), and, thus, we may assume $\lambda_0 = 1$ below.

The minimum principle yields $u(t) = -\lambda_2(t)$. Now, the following conclusions can be drawn:

LEMMA 2.1. (a) *On a free subinterval $I_f = [\tau_1, \tau_2]$ the solution $x(t) = y_1(t)$ (first component of the vector y) is a cubic C^2-spline with* *respect to the given interpolation data. If* $g[t_1], g[t_n] < 0$, *the* natural boundary conditions $y_1''(t_1) = y_1''(t_n) = 0$ *are satisfied.*

(b) *At each contact point* $\tau \notin I_0$ *the solution* x *is arbitrarily smooth* (C^∞), *at a contact point* $t_j \in I_0$ *which coincides with an interpolation knot, the solution* x *is at least* C^2, *i.e., there do not exist nontrivial contact points.*

(c) *On a boundary subarc* $I_b = [\tau_1, \tau_2]$ *the solution* x *is an affine-linear function and it is twice continuously differentiable at the junction points* τ_j, $j = 1, 2$. *If* I_b *contains no interpolation grid point,* $u'(\tau_1^-) = u'(\tau_2^+)$ *holds.*

Proof. Property (a) follows from the differential equations (with $\eta(t) = 0$, cf. (2.10)) $y_1'(t) = y_2(t)$, $y_1''(t) = u(t) = -\lambda_2(t)$, $y_1'''(t) = \lambda_1(t)$, and $y_1^{(4)}(t) = 0$. At interpolation grid points $t_j \in \text{int}(I_f)$ the second derivative $y_1'' = -\lambda_2$ is continuous ($\alpha_j = 0$ due to (2.10)), whereas $y_1''' = \lambda_1$ may have a jump discontinuity.

A contact point τ establishes a strict local minimum of y_2. Therefore, one obtains the inequalties $y_1''(\tau^-) \leqslant 0 \leqslant y_1''(\tau^+)$. On the other hand, from Eq. (2.14) and $\mu(\tau) \geqslant 0$ it follows that $y_1''(\tau^+) = -\lambda_2(\tau^+) \leqslant -\lambda_2(\tau^-) = y_1''(\tau^-)$. Thus, the control $u = y_1''$ is continuous at the contact point, and $\mu(\tau) = u(\tau) = 0$. The same derivation holds, if $\tau = t_j \in I_0$ is a contact point: Due to $\alpha_j > 0$ one obtains $\alpha_j = 0, x''(t_j) = 0$. Note that in this case the natural boundary conditions are satisfied as well.

We remark that statement (b) agrees with a more general result of Jacobson *et al.* [12] for optimal control problems with regular Hamiltonian and first order state constraints. See also Maurer and Gillessen [13].

The first statement of (c) follows from $g[t] = x'_{\min} - y_2(t) \equiv 0$ on I_b. By differentiation one obtains $y_1''(t) = u(t) = -\lambda_2(t) \equiv 0$. Therefore, $\alpha_j = 0$ holds for all knots $t_j \in \text{int}(I_b)$.

At the junction points τ_1, τ_2 the minimum property of y_1' yields $y_1''(\tau_1^-) \leqslant 0$, $y_1''(\tau_2^+) \geqslant 0$. Thus, if $\tau_1, \tau_2 \notin I_0$, Eq. (2.14) results in $0 = y_1''(\tau_1^+) = -y_1''(\tau_1^-) + \mu(\tau_1)$, which shows that $u = y_1''$ is continuous at τ_1. The same holds with respect to the other junction point τ_2. Also, the same derivation remains true, if $\tau_1 \in I_0$ or if $\tau_2 \in I_0$, because of $\alpha_j \geqslant 0$. Therefore, x is twice continuously differentiable at the junction points.

A further differentiation of $u(t) = -\lambda_2(t) \equiv 0$ reveals $\eta(t) = \lambda_1(t) \geqslant 0$, ($t \in I_b$). As λ_1 is piecewise constant with jumps only at the interpolation knots, it follows in case $I_b \cap I_0 = \varnothing$ that

$$u'(t) = -\lambda_2'(t) = \begin{cases} \lambda_1 = \text{const.} \geqslant 0, & \text{if} \quad t \in [t_j, \tau_1[, \\ 0, & \text{if} \quad t \in [\tau_1, \tau_2], \\ \lambda_1, & \text{if} \quad t \in]\tau_2, t_{j+1}]. \end{cases}$$

From this we find $u'(\tau_1^-)=u'(\tau_2^+)\geqslant 0$, and, due to the maximality property of the boundary subarc, even $u'(\tau_1^-)=u'(\tau_2^+)>0$. ∎

Note that the natural boundary conditions also hold if the t_1 or t_n are endpoints of boundary subarcs.

It may be recalled that, according to the assumption (1.5), each boundary subarc I_b contains at most one interpolation grid point. On the other hand, due to the monotone behaviour of u just described, each interpolation subinterval $[t_j, t_{j+1}]$ contains at most one boundary subarc and further between two boundary subarcs there are at least two knots of the interpolation grid.

Now, we can summarize the previous results as follows.

THEOREM 2.1. *Let x be a solution of Problem* 1.1, *i.e., x is a minimizer of the functional J subject to the interpolation and monotonicity constraints. Then x has the following properties*:

(a) *x is a natural cubic C^2 spline with respect to an augmented grid*

$$a=\tau_1<\tau_2<\cdots<\tau_N=b,$$

where the τ's consist of the given interpolation knots t_j and possibly some new knots (*to be called additional knots in the sequel*), *which are endpoints of subintervals with $x'(t)\equiv x'_{\min}$. The natural boundary conditions hold*

$$x''(t_1)=x''(t_n)=0. \tag{2.15}$$

(b) *Between two neighboring interpolation knots t_j, t_{j+1} there are at most two additional knots. If there is precisely one additional knot τ between t_j, t_{j+1}, then $x'_{\min}-x'$ vanishes either in $[t_j, \tau]$ or in $[\tau, t_{j+1}]$. If there are precisely two additional knots τ_1, τ_2 between t_j, t_{j+1}, then $x'_{\min}-x'$ vanishes between these additional knots, and*

$$x'''(\tau_1^-)=x'''(\tau_2^+)>0. \tag{2.16}$$

COROLLARY 2.1. *Analogous properties as given in Theorem* 2.1 *with the exception of the natural boundary conditions* (2.15) *hold for the solution of Problem* 1.2. *Also for Problem* 1.3 *analogous properties are valid.*

3. LOCAL, MONOTONE CUBIC SPLINE INTERPOLATION

Theorem 2.1 gives a complete characterization of optimal monotone cubic splines. For numerical purposes however, it is necessary to obtain some information, or at least a good estimate, of the number and the relative position of the additional knots with respect to the original grid. This information about the *solution structure* is not easy to obtain from the above theorem.

Therefore, it is reasonable to consider the problem for one subinterval and for boundary data of the type (1.5) taken from the unrestricted interpolating spline. We call this problem the *local problem*. It is much easier than the general one, and one can solve it essentially analytically, i.e., in terms of few nonlinear equations which have polynomial form, thus obtaining suitable initial estimates for the global problem.

In the case of a non-negative constraint this concept has been applied successfully by Dauner and Reinsch [5] and independently by Fischer *et al.* [7] for cubic spline interpolation and recently was extended to quintic splines by Oberle and Opfer [16] where some new phenomena were observed.

In the case of the monotonicity constraint (1.4) considered in this paper, the local problem is more complicated due to the fact that a boundary subarc may involve more than one subinterval of the original interpolation grid. Further, the unrestricted spline does not necessarily produce slopes $x'(t_j) > x'_{\min}$. Therefore, it does not suffice to consider only one subinterval for the local problem. However, according to the assumption (1.5), one does not need to consider more than two subintervals of the original grid. So, in the following we investigate the cases of one and two subintervals separately.

For reasons of simplicity, we restrict ourself in the following to the case $x'_{\min} = 0$. This can be done without loss of generality by the simple transformation $\tilde{x}(t) := x(t) - x'_{\min} \cdot t$.

3.1. *Case of One Subinterval*

We start with Problem 1.2 for the special case of one subinterval ($n = 2$).

Problem 3.1. For given data $t_1, t_2, x_1, x_2, b_1, b_2$ satisfying the assumptions

$$t_1 < t_2, \qquad x_1 < x_2, \qquad \text{and} \qquad b_1, b_2 > 0,$$

a continuously differentiable and piecewise smooth function x is to be determined, which minimizes the functional J subject to the constraints

$$x(t_i) = x_i, \qquad x'(t_i) = b_i \quad (i = 1, 2), \quad x'(t) \geqslant 0 \quad (t_1 \leqslant t \leqslant t_2).$$

Problem 3.1 has a unique solution. This is either the cubic Hermite interpolant for the given interpolation data if it satisfies the monotonicity constraint, or it is a cubic spline with two additional knots and one (interior) boundary subarc. The details are given in the following theorem.

THEOREM 3.1. (a) *The (unrestricted) cubic Hermite interpolation polynomial* x_0 *violates the monotonicity constraint* $x_0'(t) \geqslant 0$, *if and only if the following three inequalities are (simultaneously) satisfied,*

$$\begin{aligned} &\text{(i)} \quad u := 2b_1 + b_2 - 3x[t_l, t_2] > 0, \\ &\text{(ii)} \quad v := b_1 + 2b_2 - 3x[t_l, t_2] > 0, \\ &\text{(iii)} \quad u^2 > b_1(u+v), \end{aligned} \tag{3.1}$$

where $x[t_1, t_2] := (x_2 - x_1)/(t_2 - t_1)$ *denotes the first divided difference. If one of the inequalities* (3.1) *is not satisfied,* x_0 *is the solution of Problem* 3.1.

(b) *The conditions* (3.1) *are equivalent to the inequality*

$$z := b_1 + b_2 - 3x[t_1, t_2] > \sqrt{b_1 b_2}. \tag{3.2}$$

(c) *If the inequalities* (3.1) *are satisfied, the solution to Problem* 3.1 *is a cubic* C^2*-spline with two additional knots* τ_l, τ_2 *satisfying* $t_1 < \tau_l < \tau_2 < t_2$. *The interval* $[\tau_1, \tau_2]$ *is a boundary subarc of the monotonicity constraint. The additional knots and the corresponding interpolation data are given by the formulae*

$$\begin{aligned} \tau_1 &= t_1 + 3\frac{\sqrt{b_1}}{\sqrt{b_1^3} + \sqrt{b_2^3}}(x_2 - x_1), \\ \tau_2 &= t_2 - 3\frac{\sqrt{b_2}}{\sqrt{b_1^3} + \sqrt{b_2^3}}(x_2 - x_1), \\ x(\tau_1) &= x_1 + \frac{1}{3}b_1(\tau_1 - t_1), \\ x(\tau_2) &= x_2 + \frac{1}{3}b_2(\tau_2 - t_2). \end{aligned} \tag{3.3}$$

Proof. The unrestricted cubic Hermite interpolation polynomial x_0 can be written in the Taylor-form

$$x_0(t) = x_1 + b_1(t - t_1) + c(t - t_1)^2 + d(t - t_1)^3,$$

where $c = (-2b_1 - b_2 + 3x[t_1, t_2])/(t_2 - t_1)$ and $d = (b_1 + b_2 - 2x[t_1, t_2])/(t_2 - t_1)^2$. Now, a simple calculation shows that condition (3.1)(i) is equivalent to $x_0''(t_1) < 0$, and that condition (3.1)(ii) is equivalent to $x_0''(t_2) > 0$. Both conditions are necessary and sufficient for x' possessing a strict global minimum at some point $t_e \in]t_l, t_2[$. Now, (3.1)(iii) is equivalent to $x'(t_e) < 0$. This proves part (a) of the theorem.

The proof of part (b) is straightforward. We refer to Podewski *et al.* [18].

If Eqs. (3.1) are satisfied, Theorem 2.1 shows that the solution of Problem 3.1 is a cubic C^2-spline x with two additional knots and precisely one boundary subarc $[\tau_1, \tau_2]$. Because $x'_{\min} = 0$, this is characterized by the conditions

$$x'|_{[\tau_1, \tau_2]} = 0, \qquad x''|_{[\tau_1, \tau_2]} = 0, \qquad x'''(\tau_1^-) = x'''(\tau_2^+) > 0. \tag{3.4}$$

Therefore, by cutting off the boundary subarc, one obtains the transformed spline

$$\tilde{x}(t) := \begin{cases} x(t), & \text{if } \; t_1 \leqslant t \leqslant \tau_1, \\ x(t + \tau_2 - \tau_1), & \text{if } \; \tau_1 \leqslant t \leqslant \tilde{t}_2 := t_2 - \tau_2 + \tau_1, \end{cases} \tag{3.5}$$

which is *one* cubic polynomial corresponding to the interpolation data

$$\tilde{x}(t_1) = x_1, \qquad \tilde{x}'(t_1) = b_1, \qquad \tilde{x}(\tilde{t}_2) = x_2, \qquad \tilde{x}'(\tilde{t}_2) = b_2.$$

Further, $\tilde{x}$ fulfills the additional conditions $\tilde{x}'(\tau_1) = \tilde{x}''(\tau_1) = 0$, $\tilde{x}'''(\tau_1) > 0$. Thus, the function $\tilde{x}$ has a representation of the form $\tilde{x}(t) = a(t - \tau_1)^3 + \tilde{x}(\tau_1)$, $a > 0$. By substitution of the interpolation conditions and eliminating the parameters a and $\tilde{x}(\tau_1)$, one obtains the following nonlinear system of equations,

$$\begin{aligned} b_2 h_2 - b_1 h_1 &= 3(x_2 - x_1), \\ b_1 h_2^2 - b_2 h_1^2 &= 0 \end{aligned} \tag{3.6}$$

for the unknowns $h_1 := t_1 - \tau_1 < 0$ and $h_2 := \tilde{t}_2 - \tau_1 = t_2 - \tau_2 > 0$. Solving these equations one obtains the unique solution given in Eq. (3.3).

Obviously $\tau_1 > t_1$ and $\tau_2 < t_2$ hold. To complete the proof, we have to show that, under the assumption (3.1), $\tau_1 < \tau_2$ also holds. Elementary manipulation gives the length of the boundary subarc

$$\tau_2 - \tau_1 = (t_2 - t_1) \cdot \left(1 - \frac{3x[t_1, t_2]}{b_1 + b_2 - \sqrt{b_1 b_2}}\right). \tag{3.7}$$

Thus, $\tau_1 < \tau_2$ is equivalent to the condition (3.2), which proves part (c) of the Theorem. ▮

3.2. *Case of Two Subintervals*

Now, we consider Problem 1.2 for $n = 3$. It turns out that one can reduce this problem to one convex polynomial equation of fourth degree, which can easily be solved, say by Newton's method.

Problem 3.2. For given data (t_j, x_j), $j=1, 2, 3$, and values b_1, b_3 satisfying the assumptions

$$t_1 < t_2 < t_3, \qquad x_1 < x_2 < x_3, \qquad \text{and} \qquad b_1, b_3 > 0,$$

a continuously differentiable and piecewise smooth function x has to be determined, which minimizes the functional J subject to the interpolation conditions

$$x(t_i) = x_i \quad (i=1, 2, 3), \qquad x'(t_i) = b_i \quad (i=1, 3), \tag{3.8}$$

and the monotonicity constraint

$$x'(t) \geqslant 0 \qquad (t_l \leqslant t \leqslant t_3). \tag{3.9}$$

First, the unrestricted cubic spline x_0 corresponding to (3.8) is considered and a criterion is derived, which tells us whether x_0 satisfies the constraint (3.9) or not.

THEOREM 3.2. *Let x_0 be the unrestricted cubic spline satisfying* (3.8). *We use the abbreviations* $h_j := t_{j+1} - t_j$, $x[t_j, t_{j+1}] := (x_{j+l} - x_j)/h_j (j=1, 2)$, *and*

$$\delta_1 := 3x[t_1, t_2] - b_1, \qquad \delta_2 := 3x[t_2, t_3] - b_3. \tag{3.10}$$

The spline x_0 violates the constraint (3.9) *if and only if one of the following two conditions is satisfied*

$$\begin{aligned} &\text{(I)} \quad b_2^0 < 0, \\ &\text{(II)} \quad b_2^0 > 0, \qquad \textit{and either} \\ &\qquad z_1 := b_2^0 - \delta_1 > \sqrt{b_1 b_2^0}, \qquad \textit{or} \quad z_2 := b_2^0 - \delta_2 > \sqrt{b_2^0 b_3}, \end{aligned} \tag{3.11}$$

where

$$b_2^0 := x_0'(t_2) = \frac{\delta_1 h_2 + \delta_2 h_1}{2(h_1 + h_2)} \tag{3.12}$$

denotes the derivative of x_0 at the middle knot t_2.

Proof. The unrestricted cubic spline x_0 satisfying (3.9) may have the representation

$$x_0(t) = x_j + b_j(t - t_j) + c_j(t - t_j)^2 + d_j(t - t_j)^3, \qquad t_j < t < t_{j+1},\ j = 1, 2,$$

where $c_j = (-2b_j - b_{j+1} + 3x[t_j, t_{j+1}])/h_j$, $d_j = (b_j + b_{j+1} - 2x[t_j, t_{j+1}])/h_j^2$. In these formulae $b_2 = b_2^0$ can be determined by using the continuity of x_0'' at t_2. A simple calculation reveals (3.12).

Obviously, x_0 violates the monotonicity constraint if $x_0'(t_2) =: b_2^0 < 0$, i.e., (3.11)(I) holds. If $b_2^0 = 0$ holds, the constraint is violated if and only if $x_0''(t_2) = 2\delta_2/h_2 \neq 0$. This corresponds to (3.11)(II).

In the case $b_2^0 > 0$, one can apply Theorem 3.1 to each subinterval $[t_1, t_2]$ and $[t_2, t_3]$ which proves the condition (3.11) (II). Note that in this case the constraint (3.9) is violated in at most one subinterval mentioned. ∎

In the following theorem we classify the structure of the optimal spline with respect to its dependence on the parameters δ_1, δ_2, cf. (3.10). For reasons of conciseness we omit the technical proof of this theorem, which in principle, however, is similar to the proof of Theorem 3.1. The details may be found in Podewski *et al.* [18].

THEOREM 3.3. *We keep the notions introduced in Theorem* 3.2 *and we assume that the unrestricted spline violates the monotonicity constraint, i.e., the condition* (3.11) *holds.*

(a) *In the case $\delta_1 \leqslant 0$, $\delta_2 \leqslant 0$, and $\delta_1 + \delta_2 \neq 0$, the solution x of Problem* 3.2 *is a C^2-spline with one boundary subarc $[\tau_1, \tau_2]$. This boundary subarc includes the middle interpolation knot t_2. Explicitly, one obtains*

$$\tau_1 = t_2 + \delta_1 h_1/b_1, \qquad \tau_2 = t_2 - \delta_2 h_2/b_3, \qquad x(\tau_1) = x(\tau_2) = x_2. \tag{3.13}$$

(b) *In the case $\delta_1 > 0$ and $\delta_1 > \delta_2$, the solution x of Problem* 3.2 *is a C^2-spline with one boundary subarc $[\tau_1, \tau_2]$ which is located fully in the right subinterval, i.e., $t_2 < \tau_1 < \tau_2 < t_3$. More precisely, if u^* denotes the* (*uniquely determined*) *positive root of the polynomial* (*r stands for right*)

$$F_r(u) := \frac{h_1}{3} u^4 + 2(x_3 - x_2)\, u^2 + \frac{h_1}{3} \sqrt{b_3^3}\, u - \delta_1(x_3 - x_2), \tag{3.14}$$

then the derivative at the middle interpolation knot is given by $b_2 = x'(t_2) = (u^*)^2$, and the additional knots and the corresponding interpolation data can be determined as in Theorem 3.1, *namely*

$$\begin{aligned} \tau_1 &= t_2 + 3\,\frac{\sqrt{b_2}}{\sqrt{b_2^3}+\sqrt{b_3^3}}\,(x_3 - x_2), \\ \tau_2 &= t_3 - 3\,\frac{\sqrt{b_3}}{\sqrt{b_2^3}+\sqrt{b_3^3}}\,(x_3 - x_2), \\ x(\tau_1) &= x_2 + \frac{1}{3}\,b_2(\tau_1 - t_2), \\ x(\tau_2) &= x_3 + \frac{1}{3}\,b_3(\tau_2 - t_3). \end{aligned} \tag{3.15}$$

(c) *The analogous property holds in the case* $\delta_2 > 0$, *and* $\delta_2 > \delta_1$. *Here, the solution has one boundary subarc* $[\tau_1, \tau_2]$ *which is located in the left open subinterval* $]t_1, t_2[$. *The derivative* $b_2 = x'(t_2)$ *is given as the square of the uniquely determined positive root of the polynomial* (l *stands for left*)

$$F_l(u) := \frac{h_2}{3}\,u^4 + 2(x_2 - x_1)\,u^2 + \frac{h_2}{3}\sqrt{b_1^3}\,u - \delta_2(x_2 - x_1). \tag{3.16}$$

The additional knots τ_1, τ_2 *are given as in Theorem* 3.1 *by the formulae* (3.3).

EXAMPLE 3.1. We choose the interpolation data

$$(t_1, x_1) = (-3, -1), \quad (t_2, x_2) = (-1, 0), \quad (t_3, x_3) = (2, 3); \quad b_1 = 2,\, b_3 = 7.$$

Figure 3.1 shows the unrestricted and the optimal monotone spline of this example obtained by Theorem 3.3(a). The derivatives of the splines are given in the figure on the right. The optimal spline contains one boundary subarc with an interior interpolation knot. The additional knots, entry- and exit-points of the boundary subarc are found to be

$$\tau_1 = -1.5000000, \qquad \tau_2 = 0.71428571.$$

EXAMPLE 3.2. We choose the interpolation data

$$(t_1, x_1) = (-3, -1), \qquad (t_2, x_2) = (-1, 0), \qquad (t_3, x_3) = (2, 3);$$

$$b_1 = 0.3,\, b_3 = 4.5.$$

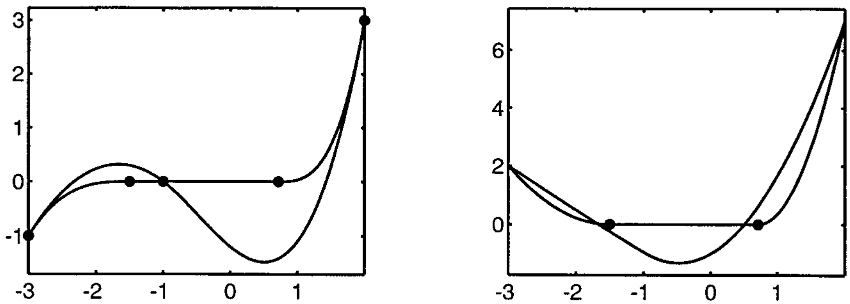

FIG. 3.1. Example 3.1; unrestricted and monotone splines and their derivatives.

Figure 3.2 shows the unrestricted spline as well as the solution obtained by Theorem 3.3(b) and its derivatives (figure on the right). The optimal monotone spline contains one boundary subarc situated in the right subinterval $[t_2, t_3]$.

The numerical figures for entry and exit point are given by

$$\tau_1 = -0.61915382, \qquad \tau_2 = 0.014005307;$$

the corresponding interpolation values are found to be $x(\tau_1) = x(\tau_2) = 0.021007961$.

Note that by the Theorem 3.3 we have obtained a complete description of the solution of Problem 3.2. First, by the condition (3.12) of Theorem 3.2, one can find out whether the unrestricted spline already solves the problem. If this is not the case, then exactly one of the three cases considered in Theorem 3.3 is valid and the corresponding restricted spline can be evaluated either directly (Theorem 3.3(a)) or by the solution of a simple polynomial equation (Theorem 3.3(b),(c)).

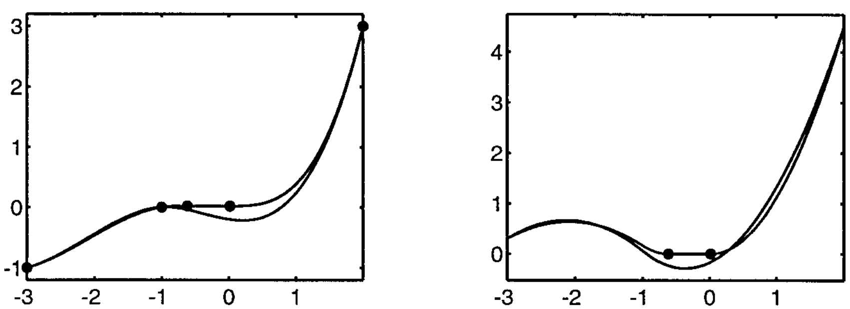

FIG. 3.2. Example 3.2; unrestricted and monotone splines and their derivatives.

4. A NUMERICAL ALGORITHM AND EXAMPLES

In this section we describe an algorithm for the numerical computation of monotone cubic splines. The algorithm is based on the necessary conditions developed in Section 2.

It is obvious that the method can be applied to more general obstacles of the form

$$x'_{\min} \leqslant x'(t) \leqslant x'_{\max}, \tag{4.1}$$

even if $x'_{\min}$, $x'_{\max}$ are replaced by step functions where the jumps may occur at the grid points of the mesh (1.3). So, for example, a switching of the constraint from monotone increasing to monotone decreasing or vice versa, can be treated as well (so-called *comonotone* cases). For simplicity we restrict the description of the algorithm to the monotone case.

The basic idea of the algorithm is given by cutting off the boundary subarcs as it is described in Eq. (3.5). Here, for each boundary subarc $[\tau_1, \tau_2]$ the spline for $t \geqslant \tau_1$ and all interpolation knots $t_j > \tau_2$ are shifted by the length of the boundary subarc $\ell := \tau_2 - \tau_1$ to the left. Thus, one obtains an *unrestricted* C^2-spline $\tilde{x}$ with respect to the modified grid for which the derivative $\tilde{x}'$ has a minimum at $t_e = \tau_1$ with $\tilde{x}'(t_e) = 0$. Thus, the spline $\tilde{x}$ can be computed by any standard algorithm for cubic spline interpolation, see, for example, Bulirsch and Rutishauser [3].

For one boundary subarc situated in the subinterval $[t_k, t_{k+1}]$, $k \in \{1, ..., n-1\}$, the transformation is given by

$$\tilde{x}(t) := \begin{cases} x(t), & \text{if} \quad t_1 \leqslant t \leqslant \tau_1, \\ x(t + \tau_2 - \tau_1), & \text{if} \quad \tau_1 \leqslant t \leqslant \tilde{t}_n, \end{cases} \tag{4.2}$$

$$\tilde{t}_j := \begin{cases} t_j, & \text{if} \quad j = 1, ..., k, \\ t_j - (\tau_2 - \tau_1), & \text{if} \quad j = k+1, ..., n. \end{cases} \tag{4.3}$$

Note that for general values of $x'_{\min}$, the ordinates of the interpolation data have to be transformed by $\tilde{x}_j = x_j - x'_{\min} \cdot \ell$, $j > k$, too, where $\ell = \tau_2 - \tau_1$ denotes the length of the boundary subarc.

For the numerical computation of the restricted spline one can proceed as follows:

For an estimate of the length ℓ of the boundary subarc one determines the shifted grid $(\tilde{t}_j)$, $(\tilde{x}_j)$ according to the above formulae. The corresponding unrestricted spline is denoted by $\tilde{x}(t, \ell)$. Now, a point $t_e(\ell) \in [\tilde{t}_k, \tilde{t}_{k+1}]$ has to be determined, where the derivative $\tilde{x}'(t, \ell)$ takes its minimum value with respect to this subinterval.

In general, $t_e(\ell)$ is situated in the interior of the interpolation interval, but sometimes it may also be situated at the endpoints $\tilde{t}_k, \tilde{t}_{k+1}$. This is the case, if the boundary subarc contains an interior interpolation knot.

The parameter ℓ has eventually to be determined such that

$$\Phi(\ell) := \tilde{x}'(t_e(\ell), \ell) = 0. \tag{4.4}$$

This can be done by means of Newton's method using the given estimate for ℓ as the starting value.

The same method works, if the restricted spline contains several boundary subarcs. In this case one has to perform the transformation (4.2), (4.3) for each boundary subarc, ℓ becomes a vector with length equal to the number of boundary subarcs, say m, and $\mathbf{\Phi}$ becomes a vector-valued function of the form

$$\mathbf{\Phi}(\ell) := \begin{pmatrix} \tilde{x}'(t_e^{(1)}(\ell), \ell) \\ \vdots \\ \tilde{x}'(t_e^{(m)}(\ell), \ell) \end{pmatrix} = \mathbf{0}, \tag{4.5}$$

where $t_e^{(k)}$ denotes the minimum of $\tilde{x}$ on the subinterval which contains the kth boundary subarc. The Jacobian of $\mathbf{\Phi}$ is computed by numerical differentiation.

After numerical convergence of the method, the computed spline $\tilde{x}$ has to be retransformed in order to obtain the restricted spline for the original problem. To this end, the additional knots are computed according to

$$\tau_1^{(k)} = t_e^{(k)}(\ell), \qquad \tau_2^{(k)} = \tau_1^{(k)} + \ell_k. \tag{4.6}$$

We note that the numerical behaviour of the method depends strongly on a suitable choice of the initial estimates. We have found that favourable initial estimations can be gained by the local monotone spline described in Section 3. The derivatives necessary for the computation of the local spline are obtained by the corresponding unrestricted spline which is determined a priori. Now, in each subinterval $[t_i, t_{i+1}]$ with $x'(t_j) > 0$, $j = i, i+1$, Theorem 3.1 is used to check whether the unrestricted spline satisfies the monotonicity constraint or not. In the latter case, Theorem 3.1 gives an explicit formula for the additional knots of the (locally) constrained spline. These are used as initial data for the computation of the globally constrained spline. The same can be done if one of the derivatives, say $x'(t_{i+1})$, is nonpositive. In this case we assume that $x'(t_j) > 0$, $j = i, i+2$, and we apply Theorem 3.3 in order to compute the additional knots (in $[t_i, t_{i+2}]$) for the locally constrained spline.

In general the number of required Newton steps to solve the problem is reduced considerably by this choice of the initial data. Further, even for stringent restrictions, the problem could be solved without applying a homotopy or continuation method. We demonstrate the behaviour of the algorithm by two examples from the literature.

EXAMPLE 4.1 (Fritsch and Carlson [8]). We choose $n = 9$ and interpolation data which are taken from a radio-chemical problem, see Table 4.1.

The data are monotone; however, the unrestricted spline is not. The optimal monotone spline has three boundary subarcs which are situated in the first, the sixth, and in the last subinterval. The entry-point of the first and the exit-point of the last boundary subarc coincides with an interpolation knot.

For this example one observes that the solution structure depends strongly on the restrictions. So, for mild restrictions $x'_{\min} < 0.118$, the solution has only one boundary subarc situated in the subinterval [10, 12].

For more stringent constraints $-0.118 < x'_{\min} < -0.00025$ a second (very small) boundary subarc in the first interval appears, which for reasons of clarity is not indicated in Fig. 4.1. For constraints $x'_{\min} > -0.00025$ a third boundary subarc exists in the last subinterval [15, 20]. For the monotone case the boundary subarcs are given in Table 4.2.

EXAMPLE 4.2. We choose $n = 8$ and interpolation data similar to an example of Späth [20, p. 102, Fig. 4.11], see Table 4.3.

The function values are monotone increasing in the interval [0, 10] and monotone decreasing in [10, 20]. Therefore, we determine an interpolating spline which preserves these properties, i.e., we use the restrictions $x'(t) \geqslant 0$ on [0, 10] and $x'(t) \leqslant 0$ on the other part [10, 20]. The algorithm solves this problem within a few Newton-steps. In Fig. 4.2 the unrestricted and the restricted splines are shown as well as their first derivatives (the figure

TABLE 4.1

Given Interpolation Data

t_j	7.99	8.09	8.19	8.7	9.2	10
x_j	0	2.76429E-5	4.37498E-2	0.169183	0.469428	0.943740
t_j	12	15	20			
x_j	0.998636	0.999919	0.999994			

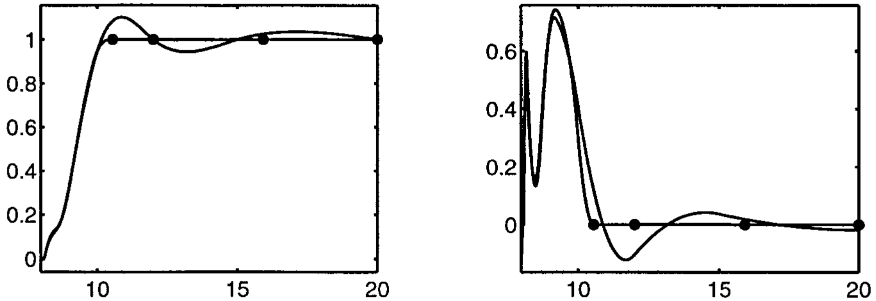

FIG. 4.1. Example 4.1; unrestricted and monotone splines and their derivatives.

TABLE 4.2

Junction Points of Example 4.1

τ_j	7.9900000	8.0865338	10.549942	11.999650	15.921658	20.000000
$x(\tau_j)$	0.0000000	0.0000000	0.9986360	0.9986360	0.9999940	0.9999940

TABLE 4.3

Interpolation Data

t_j	0	4	6	10	12	14	18	20
x_j	3	4	9	10	9	5	4	3

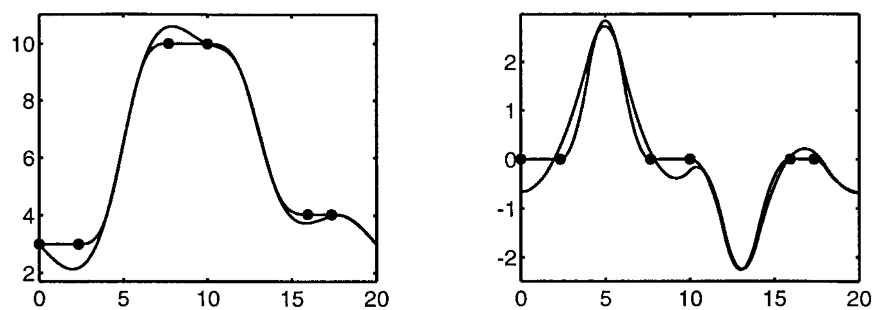

FIG. 4.2. Example 4.2; unrestricted and monotone splines and their derivatives.

TABLE 4.4

Junction Points of Example 4.2

T_j	0.0000000	2.3229670	7.6770330	10.004756	15.948384	17.354404
$x(\tau_j)$	3.0000000	3.0000000	10.000000	10.000000	4.0351027	4.0351027

on the right). The solution has three boundary subarcs. The junction points are given in Table 4.4.

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