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Reihe A	Preprints
Reihe B	Berichte
Reihe C	Mathematische Modelle und Simulation
Reihe D	Elektrische Netzwerke und Bauelemente

On the Construction of Optimal Monotone Cubic Spline Interpolation *)

Sigrid Podewski, Hans Joachim Oberle, and Gerhard Opfer

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

Abstract.

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.

*) Dedicated to Roland Bulirsch, Munich, on the occasion of his 65th birthday

1. Introduction

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

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

and given interpolation values $x_j,\ j = 1, \ldots, n,$ 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 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 (1970), Fritsch & Carlson (1980), Schmidt & Hess (1995).

The authors considered in several investigations also some kind of optimality conditions generalizing the Holladay property of the classical cubic spline, cf. Hornung (1978, 1980), Opfer & Oberle (1988, 1994), Fischer et al. (1991), Dontchev (1993) or Andersson & Elfving (1995). 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 $x_j, j = 1, 2, \ldots, n.$ We seek a minimizer x of the Holladay functional

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

subject to the constraints

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

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

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

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

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

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. The same as Problem 1.1 with additional boundary conditions for the first derivative,

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

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

Problem 1.3. The same as Problem 1 or Problem 2, however the slope is bounded also from above:

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

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* $u(t) \in \mathbb{R},\ a \le t \le b$, which minimizes the functional

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

subject to the constraints

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

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

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

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. Eq. (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. (1971) and Maurer (1979). 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 summerized as *junction points.*

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

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

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

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

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:*

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

4. *Complementarity conditions:*

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

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, Oberle (1988)), the α_j-terms occur in the Eqs. (2.9), see Chudej (1994). 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 $f_0 := u^2/2$, $f := (y_2, u)^{\mathrm{T}}$, $r_j := y_1(t_j) - x_j$, $j = 1, \ldots, n$, and $g(y) := x'_{\min} - y_2$. With these relations the augmented Hamiltonian takes the form

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

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 follows:

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

The degenerate case $\lambda_0 = 0$ can be excluded by an explicit argument: By the minimum principle the assumption $\lambda_0 = 0$ yields $\lambda_2(t) \equiv 0$ 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. (2.13–14) 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) insures 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 $t_j \in \mathrm{int}(I_f)$ 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 $y_1''(\tau^-) \leq 0 \leq y_1''(\tau^+)$. On the other hand, from Eq. (2.14) and $\mu(\tau) \geq 0$ it follows that $y_1''(\tau^+) = -\lambda_2(\tau^+) \leq -\lambda_2(\tau^-) = y_1''(\tau^-)$. 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 $\alpha_j \geq 0$ 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. (1971) for optimal control problems with regular Hamiltonian and first order state constraints. See also Maurer, Gillessen (1975).

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 $t_j \in \mathrm{int}(I_b)$.

At the junction points τ_1, τ_2 the minimum property of y_1' yields $y_1''(\tau_1^-) \leq 0, y_1''(\tau_2^+) \geq 0$. Thus, if τ_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 $\alpha_j \geq 0$. Therefore, x is twice continuously differentiable at the junction points.

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

$I_b \cap I_0 = \emptyset$ that

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

From this we find $u'(\tau_1^-) = u'(\tau_2^+) \geq 0$, 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 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 & Reinsch (1989) and independently by Fischer et al. (1991) for cubic spline interpolation and recently was extended to quintic splines by Oberle & Opfer (1995) 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 must 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

$$\begin{aligned} \tilde{x}(t) &:= x(t) - x'_{\min} \cdot t, \\ \tilde{x}_i &:= x_i - x'_{\min} \cdot t_i, \\ \tilde{b}_i &:= b_i - x'_{\min}, \ i = 1, 2. \end{aligned} \tag{3.1}$$

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

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

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

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

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* $x_0'(t) \geq 0$, *if and only if the following three inequalities are* *(simultaneously) satisfied:*

$$\begin{aligned} &\text{(i)} \quad u \quad := \quad 2\,b_1 \,+\, b_2 \,-\, 3\,x[t_1,t_2] \;>\; 0,\\ &\text{(ii)} \quad v \quad := \quad b_1 \,+\, 2\,b_2 \,-\, 3\,x[t_1,t_2] \;>\; 0, \\ &\text{(iii)} \quad u^2 \;>\; b_1\,(u\,+\,v), \end{aligned} \tag{3.2}$$

where $x[t_1,t_2] := (x_2 - x_1)/(t_2 - t_1)$ *denotes the first divided difference. If one of the inequalities (3.2) is not satisfied,* x_0 *is the solution of Problem 3.1.*

b) The conditions (3.2) are equivalent to the inequality

$$z \;:=\; b_1 \,+\, b_2 \,-\, 3\,x[t_1,t_2] \;>\; \sqrt{b_1\,b_2}. \tag{3.3}$$

c) If the inequalities (3.2) are satisfied, the solution to Problem 3.1 is a cubic C^2*-spline with two additional knots* τ_1, τ_2 *satisfying* $t_1 < \tau_1 < \tau_2 < t_2$. *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 following formulae:*

$$\begin{aligned} \tau_1 &= t_1 \,+\, 3\,\frac{\sqrt{b_1}}{\sqrt{b_1^3}\,+\,\sqrt{b_2^3}}\,(x_2 - x_1),\\ \tau_2 &= t_2 \,-\, 3\,\frac{\sqrt{b_2}}{\sqrt{b_1^3}\,+\,\sqrt{b_2^3}}\,(x_2 - x_1),\\ x(\tau_1) &= x_1 \,+\, \frac{1}{3}\,b_1\,(\tau_1 - t_1),\\ x(\tau_2) &= x_2 \,-\, \frac{1}{3}\,b_2\,(t_2 - \tau_2). \end{aligned} \tag{3.4}$$

Proof: The unrestricted cubic Hermite interpolation polynomial x_0 can be written in the form

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

where $c = (-2\,b_1 \,-\, b_2 \,+\, 3\,x[t_1,t_2])/(t_2 - t_1)$ and $d = (b_1 \,+\, b_2 \,-\, 2\,x[t_1,t_2])/(t_2 - t_1)^2$. Now, a simple calculation shows, that condition (3.2) (i) is equivalent to $x_0''(t_1) < 0$, and that condition (3.2) (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 $t_e \in]t_1, t_2[$. Now, (3.3) (iii) is equivalent to $x'(t_e) < 0$. This proves part (a) of the theorem.

For part (b), one has to prove that the inequalities (3.2) imply $z := b_1 + b_2 - 3\,x[t_1,t_2] > \sqrt{b_1\,b_2}$, and vice versa. The assumption (3.2) (iii) yields

$$b_1\,(u+v) \;<\; u^2 \;=\; (b_1+z)^2$$

or by a substitution of u, v, z

$$3\,b_1^2 + 3\,b_1\,b_2 - 6\,b_1\,x[t_1,t_2] \;<\; b_1^2 + 2\,b_1\,(b_1 + b_2 - 3\,x[t_1,t_2]) + z^2.$$

Therefore, $z^2 > b_1\,b_2$, and it remains to prove that $z > 0$. If we assume $z < 0$, our previous result shows $-b_1 - b_2 + 3\,x[t_1,t_2] > \sqrt{b_1\,b_2}$. Now, property (3.2) (i) yields $2\,b_1 + b_2 > 3\,x[t_1,t_2] > b_1 + b_2 + \sqrt{b_1\,b_2}$, and, therefore, $b_1 > b_2$. But, in the same way, property (3.2) (ii) results in $b_1 + 2\,b_2 > 3\,x[t_1,t_2] > b_1 + b_2 + \sqrt{b_1\,b_2}$, i.e. $b_2 > b_1$. Thus, $z < 0$ contradicts the assumptions (3.2), and $z > 0$ holds, which proves (3.3).

The other direction of part (b) is straightforward. By the assumption (3.3) one finds $u = b_1 + z > b_1 + \sqrt{b_1\,b_2} > 0$, and $v = b_2 + z > b_2 + \sqrt{b_1\,b_2} > 0$. Further, one has $u^2 = (b_1+z)^2 > b_1^2 + 2\,b_1\,z + b_1\,b_2 = b_1\,(u+v)$.

If Eqs. (3.2) 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

$$x'|_{[\tau_1,\tau_2]} \equiv 0, \quad x''|_{[\tau_1,\tau_2]} \equiv 0, \quad x'''(\tau_1^-) = x'''(\tau_2^+) > 0. \tag{3.5}$$

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

$$\tilde{x}(t) \;:=\; \begin{cases} x(t), & \text{if } \; t_1 \le t \le \tau_1, \\ x(t+\tau_2-\tau_1), & \text{if } \; \tau_1 \le t \le \tilde{t_2} := t_2 - \tau_2 + \tau_1, \end{cases} \tag{3.6}$$

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

$$\tilde{x}(t_1) = x_1,\; \tilde{x}'(t_1) = b_1,\; \tilde{x}(\tilde{t_2}) = x_2,\; \tilde{x}'(\tilde{t_2}) = b_2.$$

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 system of equations:

$$\begin{aligned} b_2\, h_2 \;-\; b_1\, h_1 \;&=\; 3\,(x_2 - x_1), \\ b_1\, h_2^2 \;-\; b_2\, h_1^2 \;&=\; 0 \end{aligned} \tag{3.7}$$

for the unknowns $h_1 := t_1 - \tau_1 < 0$ and $h_2 := \tilde{t}_2 - \tau_1 = t_2 - \tau_2 > 0$. The Eqs. (3.7) have the following unique solution:

$$h_1 \;=\; -\,\frac{3\,\sqrt{b_1}}{\sqrt{b_1^3}\;+\;\sqrt{b_2^3}}\;(x_2 - x_1), \quad h_2 \;=\; \frac{3\,\sqrt{b_2}}{\sqrt{b_1^3}\;+\;\sqrt{b_2^3}}\;(x_2 - x_1).$$

From this, one obtains $\tau_1 = t_1 + h_1$, $\tau_2 = t_2 - h_2$ for the junction points τ_1, τ_2.

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

$$\tau_2 \;-\; \tau_1 \;=\; (t_2 - t_1)\cdot\left(1 \;-\; \frac{3\,x[t_1, t_2]}{b_1 + b_2 - \sqrt{b_1 b_2}}\right). \tag{3.8}$$

Thus, $\tau_1 < \tau_2$ is equivalent to the condition (3.3), which proves part (c) of the Theorem.

∎

Remark. If the assumptions (3.1) (i), (ii) of Theorem 3.1 are satisfied, whereas in (3.1) (iii) equality holds, the unrestricted interpolation polynomial solves the problem 3.1 with a trivial contact point t_e at the constraint, i.e. $x'(t_e) = 0$. The proof of the third part of Theorem 3.1 remains valid, however, the length of the boundary subarc becomes zero, i.e. the boundary subarc degenerates to one contact point.

Example 3.1. We choose the following interpolation data:

$$(t_1, x_1) \;=\; (-1, 0),\;\; (t_2, x_2) \;=\; (2, 3),\;\; b_1 \;=\; 1,\;\; b_2 \;=\; 7.$$

The unrestricted spline and the optimal monotone spline obtained by Theorem 3.1 are shown in Figure 3.1. In addition, the first derivatives of the splines are shown on the right part of that figure.

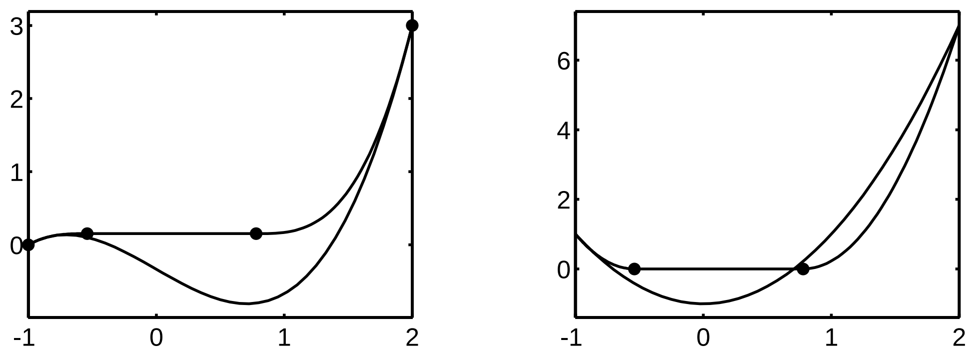

Figure 3.1.: Unrestricted and monotone splines and their derivatives.

The additional knots, entry- and exit points of the boundary subarc, are found to be

$$\tau_1 \ = \ -0.53894055, \quad \tau_2 \ = \ 0.78015135,$$

and the corresponding interpolation values are $x(\tau_1) = x(\tau_2) = 0.15368648$.

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

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

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

$$x(t_i) \ = \ x_i \ \ (i = 1, 2, 3), \quad x'(t_i) \ = \ b_i \ \ (i = 1, 3), \tag{3.9}$$

and the monotonicity constraint

$$x'(t) \geq 0 \ \ (t_1 \leq t \leq t_3). \tag{3.10}$$

First, the unrestricted cubic spline x_0 corresponding to (3.9) is considered and a criterion is derived, which tells us whether x_0 satisfies the constraint (3.10) or not.

Theorem 3.2. *Let* x_0 *be the unrestricted cubic spline satisfying (3.9). We use the abbreviations* $h_j := t_{j+1} - t_j,\ x[t_j, t_{j+1}] := (x_{j+1} - x_j)/h_j\ \ (j = 1, 2)$, *and*

$$\delta_1 := 3\,x[t_1, t_2] - b_1, \qquad \delta_2 := 3\,x[t_2, t_3] - b_3. \tag{3.11}$$

a) The derivative of x_0 *at the middle knot* t_2 *is given by*

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

b) The spline x_0 *violates the constraint (3.10) if and only if one of the following two conditions are satisfied*

(I) $b_2^0 < 0$,

(II) $b_2^0 \geq 0$, *and either* (3.13)

$$z_1 := b_2^0 - \delta_1 > \sqrt{b_1\, b_2^0}, \ \ or \ \ z_2 := b_2^0 - \delta_2 > \sqrt{b_2^0\, b_3}.$$

c) If $b_2^0 > 0$ *and* $\delta_1 > \delta_2$, *the spline* x_0 *satisfies the constraint (3.10) in the left subinterval* $[t_1, t_2]$.

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

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

where $c_j = (-2\,b_j - b_j + 3\,x[t_j, t_{j+1}])/h_j$, $d_j = (b_j + b_{j+1} - 2\,x[t_j, t_{j+1}])/h_j^2$. In these formulae $b_2 = b_2^0$ is unknown and 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. (3.13) (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 (3.13) (II). If $\delta_1 = \delta_2 = 0$, the unrestricted spline x_0 touches the constraint at the trivial contact point t_2.

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 (3.13) (II). Note that in this case the constraint (3.10) is violated in at most one subinterval.

Part (c) of the theorem is a technical statement used later on. From (3.12) one obtains

$$(2\, b_2^0 - \delta_1)\, h_2 \;=\; -\,(2\, b_2^0 - \delta_2)\, h_1.$$

As $\delta_1 > \delta_2$ holds, the left hand side of this equality must be negative. Therefore, in Theorem 3.1 the inequality (3.2) (ii) $v_1 := 2\, b_2^0 - \delta_1 > 0$ is not satisfied, i.e. the monotonicity constraint is not violated in this subinterval. ∎

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. (3.11). In Theorem 3.2 we already saw that the monotonicity constraint is inactive if $\delta_1 = \delta_2 = 0$. This remains true even if $\delta_1 = \delta_2 > 0$. This follows directly from (3.12) and (3.13) (II).

Theorem 3.3. *We keep the notions introduced in the beginning of Theorem 3.2. In the case* $\delta_1 \le 0$, $\delta_2 \le 0$, *and* $\delta_1 + \delta_2 \ne 0$, *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*

$$\tau_1 \;=\; t_2 + \delta_1\, h_1/b_1, \;\; \tau_2 \;=\; t_2 - \delta_2\, h_2/b_3, \;\; x(\tau_1) \;=\; x(\tau_2) \;=\; x_2. \tag{3.14}$$

Proof: From Theorem 3.2 one finds that the unrestricted spline violates the constraint (3.10). Therefore, the solution of Problem 3.2 has a boundary subarc. One can consider the necessary conditions for each subinterval separately. So for instance in the left subinterval $[t_1, t_2]$ we use the representation

$$x(t) \;:=\; \begin{cases} x_2 \;+\; a_1\,(t-\tau_1)^3, & \text{if} \;\; t_1 \le t \le \tau_1, \\ x_2, & \text{if} \;\; \tau_1 \;\le\; t \;\le\; t_2. \end{cases}$$

Then, the interpolation conditions at t_1 are satisfied if and only if

$$h_l \;:=\; \tau_1 \;-\; t_1 \;=\; 3\,[x_1, x_2]\, h_1/b_1 \;>\; 0, \;\; a_1 \;=\; b_1/(3\, h_l^2).$$

Further, one obtains $t_2 - \tau_1 = h_1 - h_l = h_l/b_1 \cdot (b_1 - 3\,x[t_1, t_2]) = -\delta_1\, h_1/b_1$ which shows that $\tau_1 \in\,]t_1, t_2]$.

The analogous result holds for the right subinterval and both solutions together establish a C^2-spline with one boundary subarc. Note that the entry- or the exit point of the boundary subarc coincides with t_2, if $\delta_1 = 0$ or $\delta_2 = 0$. In the limit case $\delta_1 = \delta_2 = 0$ the solution coincides with the unrestricted spline. ∎

Example 3.2. We choose the following interpolation data:

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

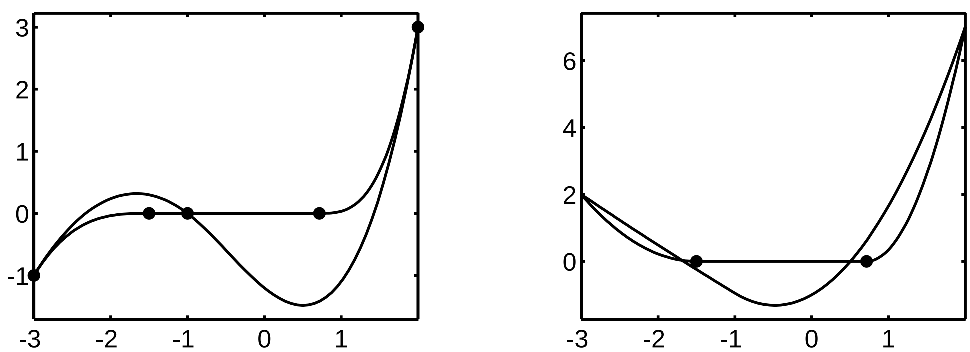

Figure 3.2.: Unrestricted and monotone splines and their derivatives.

Figure 3.2 shows the unrestricted and the optimal monotone spline of this example obtained by Theorem 3.3. 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

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

Now, we consider the more difficult situation $\delta_1 > 0$ or $\delta_2 > 0$.

Theorem 3.4. *We assume (keeping the previous notation) that the unrestricted spline violates the monotonicity constraint, i.e. the conditions (3.12) and (3.13).*

a) 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*

$$F_r(u) \;:=\; \frac{h_1}{3}\,u^4 \;+\; 2\,(x_3 - x_2)\,u^2 \;+\; \frac{h_1}{3}\,\sqrt{b_3^3}\,u \;-\; \delta_1\,(x_3 - x_2), \tag{3.15}$$

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*

$$\begin{aligned}
\tau_1 &= t_2 \;+\; 3\,\frac{\sqrt{b_2}}{\sqrt{b_2^3} \;+\; \sqrt{b_3^3}}\;(x_3 - x_2),\\
\tau_2 &= t_3 \;-\; 3\,\frac{\sqrt{b_3}}{\sqrt{b_2^3} \;+\; \sqrt{b_3^3}}\;(x_3 - x_2),\\
x(\tau_1) &= x_2 \;+\; \frac{1}{3}\,b_2\,(\tau_1 - t_2),\\
x(\tau_2) &= x_3 \;-\; \frac{1}{3}\,b_3\,(t_3 - \tau_2).
\end{aligned} \tag{3.16}$$

b) 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*

$$F_l(u) \;:=\; \frac{h_2}{3}\,u^4 \;+\; 2\,(x_2 - x_1)\,u^2 \;+\; \frac{h_2}{3}\,\sqrt{b_1^3}\,u \;-\; \delta_2\,(x_2 - x_1). \tag{3.17}$$

The additional knots τ_1, τ_2 *are given as in Theorem 3.1 by the formulae (3.4).*

Proof: Due to reasons of symmetry it suffices to prove part (a) of the Theorem. We use an ansatz for the restricted spline with one boundary subarc situated in the right subinterval. Taking into account the junction conditions and Eq. (2.16) we obtain the following representation

$$x(t) := \begin{cases} x_1 + b_1(t-t_1) + c_1(t-t_1)^2 + d_1(t-t_1)^3, & \text{if } t_1 \le t \le t_2, \\ a_2\,(t-\tau_1)^3 + x(\tau_1), & \text{if } t_2 \le t \le \tau_1, \\ x(\tau_1), & \text{if } \tau_1 \le t \le \tau_2, \\ a_2\,(t-\tau_2)^3 + x(\tau_1), & \text{if } \tau_2 \le t \le t_3. \end{cases}$$

With the variables $b_2 := x'(t_2) > 0$, $h_l := t_2 - \tau_1 < 0$, and $h_r := t_3 - \tau_2 > 0$, the interpolation conditions $x(t_j) = x_j,\, x'(t_j) = b_j,\, j = 2,3$ and the C^2-property of x lead to the following equations

$$\begin{aligned} c_1 &= (\delta_1 - b_1 - b_2)/h_1, \\ d_1 &= (b_1 + b_2 - 2\,[x_1, x_2])/h_1^2, \\ h_l &= b_2\,h_1/(2\,b_2 - \delta_1), \\ h_r &= -\sqrt{b_3/b_2}\;\,h_l, \\ a_2 &= b_2/(3\,h_l^2), \\ x(\tau_1) &= x_2 - b_2\,h_l/3, \text{ and} \\ 3(x_3 - x_2) &= -\left(b_3\sqrt{b_3/b_2} + b_2\right)\,h_l. \end{aligned} \tag{3.18}$$

By substitution of h_l from the third equation into the last one, it follows that

$$3\,(x_3 - x_2)\,(2\,b_2 - \delta_1) = -\sqrt{b_3^3}\,\sqrt{b_2}\,h_1 - b_2^2\,h_1, \tag{3.19}$$

and, therefore, with $u := \sqrt{b_2}$ we have

$$F_r(u) = \frac{h_1}{3}\,u^4 + 2\,(x_3 - x_2)\,u^2 + \frac{h_1}{3}\sqrt{b_3^3}\,u - \delta_1\,(x_3 - x_2) = 0. \tag{3.20}$$

Now, one finds $F_r'(u) \ge h_1/3\,\sqrt{b_3^3} > 0$ for all $u \ge 0$, and $F_r(0) = -\,\delta_1\,(x_3 - x_2) < 0$. This implies that Eq. (3.20) has a unique positive solution $u^* > 0$.

Further, due to $F_r(\sqrt{\delta_1/2}) = h_1\,\delta_1^2/12 + h_1/6\,\sqrt{2\,b_3^3\,\delta_1} > 0$, we find $u^* < \sqrt{\delta_1/2}$, and, with $b_2 := (u^*)^2$, it follows that $2\,b_2 < \delta_1$. Therefore, Eqs. (3.18) are satisfied and the desired sign conditions $b_2 > 0,\, h_l < 0,\, h_r > 0$ are satisfied.

It remains to prove, that the junction points $\tau_1 = t_2 - h_l$, and $\tau_2 = t_3 - h_r$ are ordered in the right way, i.e. $\tau_1 < \tau_2$. By a reformulation of h_l, h_r from Eqs. (3.18) using Eq. (3.19), we obtain the representation (3.16) for the additional knots. Therefore, the spline x restricted to the right subinterval $[t_2, t_3]$ coincides with the monotone spline x_r on the right subinterval alone, corresponding to the interpolation data $x_r(t_j) = x_j$, $x_r'(t_j) = b_j$ for $j = 2, 3$. For this spline, Theorem 3.1 can be applied, showing that $\tau_1 < \tau_2$ holds, provided the inequality (3.3) is satisfied. Here, this inequality reads

$$z_2 \;:=\; b_2 \;-\; \delta_2 \;>\; \sqrt{b_2\, b_3}. \tag{3.21}$$

Suppose Eq. (3.21) is not satisfied, i.e. according to (3.11)

$$3\, x[t_2, t_3] \;\geq\; b_2 \;+\; b_3 \;-\; \sqrt{b_2\, b_3} \;>\; 0. \tag{3.22}$$

We write $3\, x[t_2, t_3] = (1 + \alpha)\, (b_2 + b_3 - \sqrt{b_2\, b_3})$, where $\alpha \geq 0$. From Eq. (3.19) we obtain

$$\frac{\delta_1 - 2\, b_2}{h_1} \;=\; \frac{\sqrt{b_2}\, (\sqrt{b_2^3} + \sqrt{b_3^3})}{3\, x[t_2, t_3]\, h_2} \;=\; \frac{\sqrt{b_2}\, (\sqrt{b_2} + \sqrt{b_3})\, (b_2 + b_3 - \sqrt{b_2\, b_3})}{3\, x[t_2, t_3]\, h_2},$$

which, by assumption (3.22), yields

$$\frac{\delta_1}{h_1} \;=\; \frac{2\, b_2}{h_1} + \frac{b_2 \;+\; \sqrt{b_2\, b_3}}{(1 + \alpha)\, h_2}.$$

From this, the parameter δ_1 can be eliminated by means of Eq. (3.12). We obtain

$$2\left(\frac{1}{h_1} + \frac{1}{h_2}\right) b_2^0 \;=\; \frac{2\, b_2}{h_1} + \frac{b_2 \;+\; \sqrt{b_2\, b_3}}{(1 + \alpha)\, h_2} + \frac{\delta_2}{h_2}.$$

Now, a simple manipulation of this equation and the separation of the α-terms leads to

$$0 \;=\; 2\, \alpha\, \frac{b_2 - b_2^0}{h_1} + \alpha\, \frac{\delta_2 - 2\, b_2^0}{h_2} + 2\, \frac{b_2 - b_2^0}{h_1} + \frac{b_2 - b_2^0}{h_2} + \frac{\delta_2 - b_2^0 + \sqrt{b_2\, b_3}}{h_2}. \tag{3.23}$$

We consider the following two cases separately.

If $b_2^0 \geq b_2$ holds, the first four terms in the right-hand side of Eq. (3.23) are non-positive. For the second term, this follows from $\delta_1 > \delta_2$ and Eq. (3.12). So, it follows that the last term of (3.23) is non-negative, i.e. $b_2^0 \geq b_2 > 0$ and $z_2 = b_2^0 - \delta_2 \leq \sqrt{b_2\, b_3} \leq \sqrt{b_2^0\, b_3}$, cf. Eq. (3.13). By Theorem 3.2 the unrestricted spline x_0 satisfies the monotonicity constraint in the whole interval $[t_1, t_3]$ which contradicts the assumption of the theorem.

For the second case, we assume $b_2^0 < b_2$. From Eq. (3.22) we obtain $\delta_2 - b_2 + \sqrt{b_2\, b_3} = \alpha\,(b_2 + b_3 - \sqrt{b_2\, b_3})$, $\alpha \geq 0$. Substituting this into Eq. (3.23), we obtain

$$0 \;=\; 2\,\alpha\,\frac{b_2 - b_2^0}{h_1} \;+\; \alpha\,\frac{b_2 - b_2^0}{h_2} \;+\; \alpha\,\frac{3\,x[t_2, t_3] - b_2^0 - \sqrt{b_2\, b_3}}{h_2} \;+\; 2\,\frac{b_2 - b_2^0}{h_1} \;+\; 2\,\frac{b_2 - b_2^0}{h_2}\,.$$

Therefore, $\alpha > 0$ and $3\,x[t_2, t_3] - b_2^0 - \sqrt{b_2\, b_3} < 0$ hold. From the last inequality together with (3.22), it follows that $b_2 - b_2^0 + b_3 - 2\sqrt{b_2\, b_3} < 0$, i.e. $b_2^0 > (\sqrt{b_3} - \sqrt{b_2})^2 \geq 0$ and thus,

$$\sqrt{b_3} - \sqrt{b_2} \;<\; \sqrt{b_2^0} \;<\; \sqrt{b_2}\,. \tag{3.24}$$

Now, we consider the following parabola $p(t) := -t^2 + \sqrt{b_3}\,t + \delta_2$. A simple evaluation shows (cf. (3.22))

$$p(\sqrt{b_3} - \sqrt{b_2}) \;=\; p(\sqrt{b_2}) \;=\; \delta_2 + \sqrt{b_2\, b_3} - b_2 \geq 0.$$

Therefore, due to Eq. (3.24), $p(\sqrt{b_2^0}) = -b_2^0 + \sqrt{b_2^0\, b_3} + \delta_2 > 0$ holds, which shows that also in this case the unrestricted spline satisfies the monotonicity constraint which contradicts our assumption. In summary, we have shown that Eq. (3.21) is satisfied. ∎

Note that by the Theorems 3.2 – 3.4 we have obtained a complete description of the solution of Problem 3.2. First, by the conditions (3.12), (3.13) 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 the Theorems 3.3 and 3.4 is valid and the corresponding restricted spline can be evaluated either directly (Theorem 3.3) or by the solution of a simple polynomial equation (Theorem 3.4).

Example 3.3. We choose the following interpolation data:

$$(t_1, x_1) \;=\; (-3, -1),\;\; (t_2, x_2) \;=\; (-1, 0),\;\; (t_3, x_3) \;=\; (2, 3); \quad b_1 \;=\; 0.3,\;\; b_3 \;=\; 4.5.$$

Figure 3.3 shows the unrestricted spline as well as the solution obtained by Theorem 3.4 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 $x(\tau_1) = x(\tau_2) = 0.021007961$.

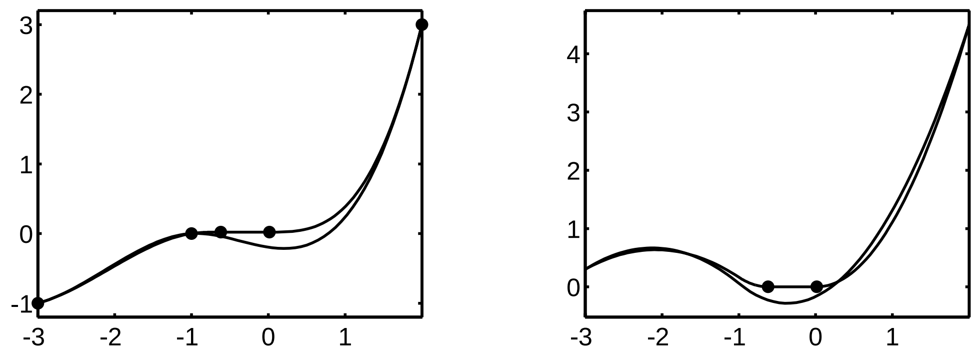

Figure 3.3.: Unrestricted and monotone splines and their derivatives.

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 for more general obstacles of the form

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

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. (3.6). Here, for each boundary subarc $[\tau_1, \tau_2]$ the spline for $t \geq \tau_1$ 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, Rutishauser (1968).

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

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

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

Note that for general values of x'_{min}, the ordinates of the interpolation data have to be transformed by $\tilde{x}_j = x_j - x'_{\text{min}} \cdot \ell \, (j > k)$, 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 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,

$\boldsymbol{\ell}$ becomes a vector which length equals the number of boundary subarcs, say m, and $\boldsymbol{\Phi}$ becomes a vector-valued function of the form

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

where $t_e^{(k)}$ denotes the minimum of $\tilde{x}$ on those subinterval which contains the k-th boundary subarc. The Jacobian of $\boldsymbol{\Phi}$ 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

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

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. 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, Carlson (1980))
We choose $n = 9$ and the following interpolation data which are taken from a radiochemical problem, see Table 4.1.

Table 4.1. Given interpolation data.

t_j	7.99	8.09	8.19	8.7	9.2	10
x_j	0	$2.76429\,e-5$	$4.37498\,e-2$	0.169183	0.469428	0.943740

t_j	12	15	20
x_j	0.998636	0.999919	0.999994

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.

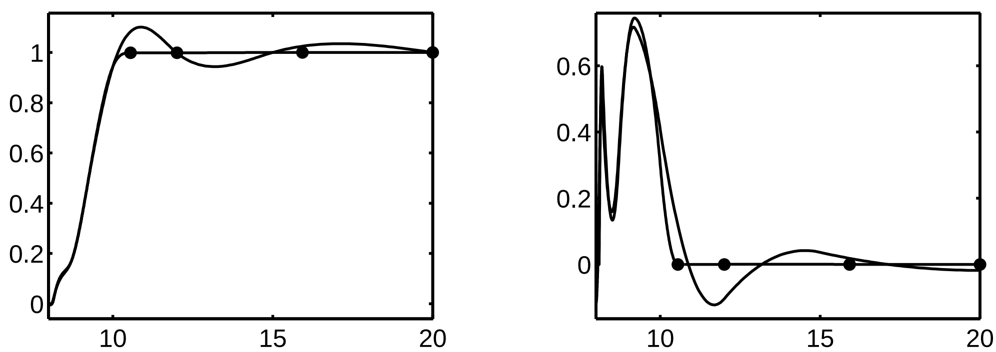

Figure 4.1.: Unrestricted and monotone splines and their derivatives.

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 Figure 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 the following Table 4.2.

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

Example 4.2.

We choose $n = 8$ and the following interpolation data similar to an example of Späth (1990, page 110, Fig. B53), see Table 4.3.

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

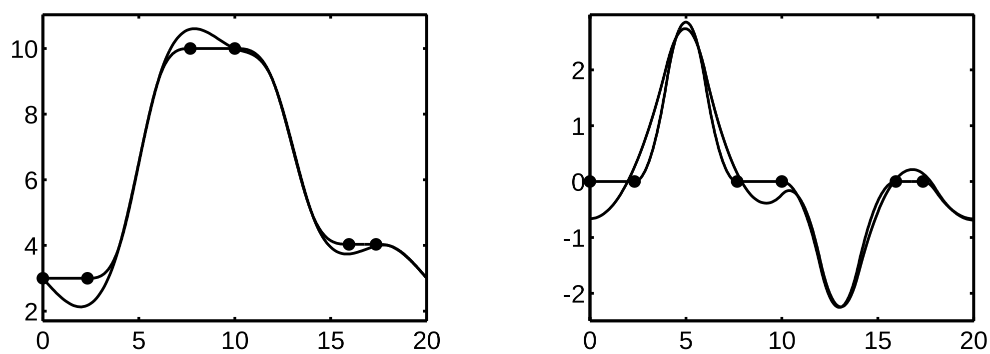

Figure 4.2.: Unrestricted and monotone splines and their derivatives.

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 $x'(t) \geq 0$ on $[0, 10]$ and $x'(t) \leq 0$ on the other part $[10, 20]$. The algorithm solves this problem within a few Newton-steps. In Figure 4.2 the unrestricted and the restricted splines are shown as well as their first derivatives (the figure on the right). The solution has three boundary subarcs. The junction points are given in the following Table 4.4.

Table 4.4. Junction points of Example 4.2.

τ_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

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