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Paper

Monotone Smoothing Spline Curves Using Normalized Uniform Cubic B-splines*

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This paper considers a problem on the non-negative derivative constraints on the cubic smoothing spline curves using normalized uniform B-splines as the basis functions. In particular, we derive a condition for monotonic constraints over interval based on the study of Fritsch and Carlon. Moreover, we present how these results are incorporated in the optimal smoothing spline problems. The performance is examined by a numerical example.

1. Introduction

The interpolating and smoothing splines have been developed as basic tools for constructing continuously differentiable curves from a given set of discrete observational data, e.g. time series data (see e.g. [1–3]). The interpolating splines are powerful tools for the cases where the data is exactly known, i.e. non-noisy data. Such cases appear, for example, in numerical analysis (e.g. [4]). However, in most practical cases, the data (e.g. some experimental data) is often corrupted by noises. Then, the smoothing splines are expected to yield more feasible solutions than interpolating splines, thus they have been widely studied in a statistical setting (e.g. [5–7]). As an example of such studies, the authors in [8] have analyzed statistical and asymptotical properties of optimal smoothing splines when the number of data increases.

In this paper we focus on a problem of constructing smoothing spline curves from noisy data. These smoothing splines are useful in real applications with statistical setting – such as non-parametric probability density estimation [9], design of digital signal (or image) filter [10,11] and human movement modeling [12]. In such cases, we often face the problems where the curves are required to preserve certain geometric properties in the given set of data, e.g. non-negativity, monotonicity and convexity, etc. For this reason, problems of the so-called constrained splines have been studied by several researchers. For example, Egerstedt et al. in [13] have considered a problem of constructing monotone smoothing splines, where the non-negativity on the derivative of splines is imposed over an interval. Such a problem leads to an infinite dimensional problem, and is formulated and solved as a dynamic programming problem. Similar problems are treated by Elfving et al. in [14] and Meyer in [15].

Recently, the authors have also considered such problems by employing B-spline approach [16,17]. Specifically, we have shown that various types of constraints can be formulated as linear constraints on the so-called ‘control points’ of B-splines, and the problems reduced to convex quadratic programming (QP) problems. Included in such constraints are equality or inequality constraints, on the function value or on its derivatives, at isolated points or over intervals, or on integral value on an interval, and their combinations. Although the conditions on the control points are simple to use, those for the constraints over interval are imposed only as sufficient conditions.

The main focus of this study is on the monotone splines, e.g. non-negative derivative constraints on the smoothing spline curves, where we consider only the cubic case. We employ normalized uniform B-splines as the basis functions. In particular, inspired by Fritsch and Carlon[18], we derive a condition for monotonic constraints over interval. Our results will be similar to those in [18] for monotone Hermite cubic interpolation, but differ in that we give a condition for the monotonicity as linear function in terms of control points. This is important since it leads to an algorithm that can be easily implemented and used in practice. Although the new condition is again sufficient, we see that it relaxes the condition developed in [17]. Moreover, we present how these results are incorporated in the optimal smoothing spline problems. The results are useful since cubic splines are most frequently used in practice. The extensions to higher

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degrees as quartic or quintic splines (e.g.[19,20]) are desirable, but their treatments are significantly different and will not be considered here.

This paper is organized as follows. In Section **2.**, we briefly present B-splines and design problem of optimal monotone smoothing splines. In Section **3.**, we review the basic problem of optimal smoothing splines, and we show how monotonic constraints on splines can be formulated and solved in Section **4.**. Then, we examine the performances of the proposed method by numerical examples in Section **5.**. Concluding remarks are given in Section **6.**.

2. Problem Statement

In this paper, we consider monotone smoothing spline curves restricting to the cubic case. We design curves $x(t)$ by employing normalized, uniform cubic B-spline function $B_3(t)$ as the basis functions,

$$x(t)=\sum_{i=-3}^{m-1}\tau_i B_3(\alpha(t-t_i)), \tag{1}$$

where m is an integer, $\tau_i\in\mathbf{R}$ is a weighting coefficients called 'control points', and $\alpha(>0)$ is a constant for scaling the interval between equally-spaced knot points t_i with

$$t_{i+1}-t_i=\frac{1}{\alpha}. \tag{2}$$

Then $x(t)$ formed in (1) is a spline of degree three with the knot points t_i. By an appropriate choice of τ_i's, arbitrary cubic spline can be designed in the interval $[t_0,t_m]$.

In (1), $B_3(t)$ is defined by

$$B_3(t)=\begin{cases}N_{3-j,3}(t-j), & j\le t<j+1,\\ & \qquad j=0,1,2,3\ .\\ 0, & t<0\ \text{ or }\ t\ge 4\end{cases} \tag{3}$$

The basis elements $N_{j,3}(t)$ $(j=0,1,2,3)$, $0\le t\le 1$ can be obtained recursively by the following improved de Boor and Cox's algorithm (see e.g. [21]).

[**Algorithm 1**] Let $N_{0,0}(t)\equiv 1$ and, for $i=1,2,3$, compute

$$\begin{cases}N_{0,i}(t) &= \dfrac{1-t}{i}N_{0,i-1}(t)\\ N_{j,i}(t) &= \dfrac{i-j+t}{i}N_{j-1,i-1}(t)\\ &\quad +\dfrac{1+j-t}{i}N_{j,i-1}(t),\ j=1,\cdots,i-1\\ N_{i,i}(t) &= \dfrac{t}{i}N_{i-1,i-1}(t).\end{cases} \tag{4}$$

Then, $N_{j,3}(t)$ are shown in Table 1 together with the derivatives. Thus, $B_3(t)$ is a piecewise cubic polynomial with integer knot points and is twice continuously differentiable. It is noted that $B_3(t)$ is normalized in the sense

Table 1 $N_{j,3}(t)$ $(j=0,\cdots,3)$ and its derivatives

	$3!N_{j,3}(t)$	$2!N_{j,3}^{(1)}(t)$	$N_{j,3}^{(2)}(t)$	$N_{j,3}^{(3)}(t)$
$j=0$	$(1-t)^3$	$-(1-t)^2$	$1-t$	-1
$j=1$	$4-6t^2+3t^3$	$-4t+3t^2$	$-2+3t$	3
$j=2$	$1+3t+3t^2-3t^3$	$1+2t-3t^2$	$1-3t$	-3
$j=3$	t^3	t^2	t	1

$$\sum_{j=0}^{3}N_{j,3}(t)=1,\ 0\le t\le 1. \tag{5}$$

If we focus on an interval $[t_j,t_{j+1}]$ $(0\le j<m)$, $x(t)$ in (1) is written as

$$x(t)=\sum_{i=-3+j}^{j}\tau_i B_3(\alpha(t-t_i)), \tag{6}$$

since, by (3), $B_3(\alpha(t-t_i))$ vanishes in $[t_j,t_{j+1}]$ for $i<-3+j$ and $i>j$.

Now, suppose that we are given a set of data

$$\mathcal{D}=\{(u_i;d_i):t_i\in[t_0,t_m],\ d_i\in\mathbf{R},\ i=1,\cdots,N\}, \tag{7}$$

and let $\tau\in\mathbf{R}^M$ $(M=m+3)$ be the control point vector defined by

$$\tau=\begin{bmatrix}\tau_{-3} & \tau_{-2} & \cdots & \tau_{m-1}\end{bmatrix}^T. \tag{8}$$

Here, we consider the following problem for designing optimal monotone smoothing splines.

[**Problem 1**] Construct the spline $x(t)$ in (1) such that

$$\min_{\tau\in\mathbf{R}^M} J(\tau)$$

subject to

$$x^{(1)}(t)\ge 0,\quad \forall t\in[t_j,t_{j+1}] \tag{9}$$

for given j $(0\le j<m)$, where

$$J(\tau)=\lambda\int_{t_0}^{t_m}\left(x^{(2)}(t)\right)^2dt+\sum_{i=1}^{N}w_i\left(x(u_i)-d_i\right)^2, \tag{10}$$

$\lambda>0$, and $w_i\in(0,1]$ $\forall i$.

(Remark 1) The above inequality '$\ge$' in (9) can be readily replaced with '$\le$' or equality '$=$', as we will see in the subsequent developments. Thus, this constraint for each knot point interval $[t_j,t_{j+1}]$ allows us more flexible control on monotonicity constraints over intervals, such as the curve being monotonically increasing on some interval and decreasing on another.

3. Optimal Smoothing Spline Curves

In this section, we first confine ourselves to express the cost function of the optimal design for the case without any constraints on $x(t)$ (see e.g. [21]).

First, in order to express (10) in terms of the vector τ in (8), we introduce $b(t)\in\mathbf{R}^M$ and a matrix $B\in\mathbf{R}^{M\times N}$ defined respectively as

$$b(t) = \left[\, B_3(\alpha(t-t_{-3}))\ B_3(\alpha(t-t_{-2}))\ \cdots \right.$$
$$\left. \cdots\ B_3(\alpha(t-t_{m-1}))\, \right]^T, \tag{11}$$
$$B = \left[\, b(u_1)\ b(u_2)\ \cdots\ b(u_N)\, \right]. \tag{12}$$

Then, noting that $x(t)$ is expressed as

$$x(t) = \tau^T b(t), \tag{13}$$

the cost function in (10) is written as quadratic function in terms of τ as

$$J(\tau) = \tau^T G\tau - 2\tau^T g + r \tag{14}$$

with

$$G = \lambda Q + BWB^T \tag{15}$$
$$g = BWd \tag{16}$$
$$r = d^T Wd, \tag{17}$$

where

$$W = \mathrm{diag}\{w_1,\ w_2,\ \cdots,\ w_N\} \tag{18}$$
$$d = \left[\, d_1\ d_2\ \cdots\ d_N\, \right]^T. \tag{19}$$

Also, $Q \in \mathbf{R}^{M\times M}$ in (15) is a Gramian defined by

$$Q = \int_{t_0}^{t_m} \frac{d^2 b(t)}{dt^2}\frac{d^2 b^T(t)}{dt^2} dt. \tag{20}$$

Once α and m in (1) are set, the Gramian Q is computed explicitly as follows (see e.g. [21]): By introducing a new integration variable

$$t' = \alpha(t-t_0), \tag{21}$$

we have $dt' = \alpha dt$. Moreover, (2) yields $\alpha(t-t_i) = t' - \alpha(t_i - t_0) = t' - i$. Then we find that

$$Q = \alpha^3 R, \tag{22}$$

where $R \in \mathbf{R}^{M\times M}$ is defined by

$$R = \int_0^m \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt, \tag{23}$$

with

$$\hat{b}(t) = [B_3(t-(-3))\ B_3(t-(-2))\ \cdots$$
$$\cdots\ B_3(t-(m-1))]^T. \tag{24}$$

Here, it can be shown that R is obtained by

$$R = R_\infty - (R_- + R_+), \tag{25}$$

where

$$R_\infty = \int_{-\infty}^{+\infty} \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt$$
$$= \frac{1}{6}\begin{bmatrix} 16 & -9 & 0 & 1 & & & & \\ -9 & 16 & -9 & 0 & 1 & & & \\ 0 & -9 & 16 & -9 & 0 & 1 & & \\ 1 & 0 & -9 & 16 & -9 & 0 & 1 & \\ & \ddots & & & \ddots & & & \ddots \\ & & \ddots & & & \ddots & & \\ & & & \ddots & & & \ddots & \\ & & & & 1 & 0 & -9 & 16 \end{bmatrix} \tag{26}$$

$$R_- = \int_{-\infty}^{0} \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt$$
$$= \frac{1}{6}\left[\begin{array}{ccc|c} 14 & -6 & 0 & \\ -6 & 8 & -3 & 0_{3,M-3} \\ 0 & -3 & 2 & \\ \hline & 0_{M-3,3} & & 0_{M-3,M-3} \end{array}\right], \tag{27}$$

$$R_+ = \int_{m}^{+\infty} \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt$$
$$= \frac{1}{6}\left[\begin{array}{c|ccc} 0_{M-3,M-3} & & 0_{M-3,3} & \\ \hline & 2 & -3 & 0 \\ 0_{3,M-3} & -3 & 8 & -6 \\ & 0 & -6 & 14 \end{array}\right]. \tag{28}$$

We see that G in (15) is positive-semidefinite, or $G \geq 0$, since $\lambda > 0$, $Q \geq 0$ and $W \geq 0$. Hence $J(\tau)$ in (14) is convex in τ. Thus, if the constraint (9) is not present in **Problem 1**, the optimal solution is given as a solution of linear algebraic equation,

$$G\tau = g. \tag{29}$$

(Remark 2) Smoothing splines can also be used to approximate given functions. In this case, the data is given as a function $f(t) \in \mathbf{R}$, $t \in [t_0, t_m]$ instead of (7), and we employ the cost function $J(\tau)$ defined by

$$J(\tau) = \lambda \int_{t_0}^{t_m} \left(x^{(2)}(t)\right)^2 dt + \int_{t_0}^{t_m} (x(t) - f(t))^2 dt. \tag{30}$$

Then, it can be shown that this cost $J(\tau)$ is also written as a convex quadratic function of τ similarly as (14).

4. Monotone Smoothing Splines

For the smoothing splines $x(t)$ in the previous section, we impose the monotonic condition (9), namely

$$x^{(1)}(t) \geq 0 \quad \forall t \in [t_j, t_{j+1}]. \tag{31}$$

Then our task is to express such constraints in terms of the control points τ_i. In the sequel, we first derive a condition for monotonic constraints based on Fritsch and Carlton's work [18] (Section **4.1**). Then, we present how such results are incorporated in the optimal smoothing spline problems (Section **4.2**).

4.1 Monotonic Conditions of Spline Curves

Since the curve $x(t)$ is a piecewise polynomial, we examine the polynomial $x(t)$ in each interval $[t_j, t_{j+1}]$ for $j = 0, 1, \cdots, m-1$.

For the interval $[t_j, t_{j+1}]$, we rewrite (6) by (3) as

$$x(t) = \sum_{i=0}^{3} \tau_{j-3+i} N_{i,3}(\alpha(t - t_j)), \quad t \in [t_j, t_{j+1}]. \tag{32}$$

Thus, we see that $x(t)$ depends on only the four weights τ_{j-3}, τ_{j-2}, τ_{j-1}, τ_j. Moreover, by introducing a new variable u,

$$u = \alpha(t - t_j), \tag{33}$$

the interval $[t_j, t_{j+1}]$ in t is normalized to $[0,1]$ in u. We then write $x(t)$ in (32) as $\hat{x}(u)$,

$$\hat{x}(u) = \sum_{i=0}^{3} \tau_{j-3+i} N_{i,3}(u), \quad u \in [0,1]. \tag{34}$$

Note here that the l-th derivative $x^{(l)}(t)$ for $t \in [t_j, t_{j+1}]$ is expressed in terms of $u \in [0,1]$ in (34) by

$$x^{(l)}(t) = \alpha^l \hat{x}^{(l)}(u), \ l = 0, 1, 2, 3, \tag{35}$$

with

$$\hat{x}^{(l)}(u) = \sum_{i=0}^{3} \tau_{j-3+i} N_{i,3}^{(l)}(u). \tag{36}$$

Using Table 1, we obtain an explicit form for $\hat{x}(u)$ in (34) as

$$\hat{x}(u) = \frac{1}{6}\left(p_j u^3 + 3 q_j u^2 + 3 r_j u + s_j\right) \tag{37}$$

with

$$p_j = \tau_j - 3\tau_{j-1} + 3\tau_{j-2} - \tau_{j-3} \tag{38}$$
$$q_j = \tau_{j-1} - 2\tau_{j-2} + \tau_{j-3} \tag{39}$$
$$r_j = \tau_{j-1} - \tau_{j-3} \tag{40}$$
$$s_j = \tau_{j-1} + 4\tau_{j-2} + \tau_{j-3}, \tag{41}$$

and thus the first derivative $\hat{x}^{(1)}(u)$ is given as

$$\hat{x}^{(1)}(u) = \frac{1}{2}\left(p_j u^2 + 2 q_j u + r_j\right). \tag{42}$$

Also, the second derivative $\hat{x}^{(2)}(u)$ is expressed as

$$\hat{x}^{(2)}(u) = p_j u + q_j. \tag{43}$$

Now we consider monotonicity constraints (31) or equivalently $\hat{x}^{(1)}(u) \geq 0 \ \forall u \in [0,1]$ for $\hat{x}(u)$ in (37). We follow the approach employed in [18], where the constraints are examined using the boundary values of the curve, i.e. $\hat{x}(0)$, $\hat{x}(1)$, $\hat{x}^{(1)}(0)$ and $\hat{x}^{(1)}(1)$ in the present case. In particular, we find the range of $\hat{x}^{(1)}(0)$ and $\hat{x}^{(1)}(1)$, in which the condition (31) holds, for each points $\hat{x}(0)$ and $\hat{x}(1)$. Note that these values can then be rewritten in terms of the four control points τ_{j-3}, τ_{j-2}, τ_{j-1}, τ_j using the following relations,

$$\begin{aligned} p_j &= 6(\hat{x}^{(1)}(1) + \hat{x}^{(1)}(0) - 2\hat{x}(1) + 2\hat{x}(0)) \\ q_j &= 2(-\hat{x}^{(1)}(1) - 2\hat{x}^{(1)}(0) + 3\hat{x}(1) - 3\hat{x}(0)) \\ r_j &= 2\hat{x}^{(1)}(0) \\ s_j &= 6\hat{x}(0). \end{aligned} \tag{44}$$

Now let $\Delta\hat{x} \in \mathbf{R}$ be the slope of the line segment between $\hat{x}(0)$ and $\hat{x}(1)$, i.e.

$$\Delta\hat{x} = \hat{x}(1) - \hat{x}(0). \tag{45}$$

Then, it is obvious that a necessary condition for monotonicity in (31) is given by

$$\hat{x}^{(1)}(0) \geq 0 \quad \hat{x}^{(1)}(1) \geq 0 \quad \Delta\hat{x} \geq 0. \tag{46}$$

In the sequel, we examine sufficient conditions assuming $\Delta\hat{x} > 0$ and then derive a necessary and sufficient condition for monotonicity. We will see that the case of $\Delta\hat{x} = 0$ is included in the theorem as a degenerate case of $\hat{x}(u) = \text{const}$.

Noting that $\hat{x}^{(1)}(u)$ in (42) is quadratic, the monotonicity is examined in the following two cases:

(P1) $p_j \leq 0$
(P2) $p_j > 0$

For the case (P1), we obtain Lemma 1.

[**Lemma 1**] Assume that (46) and (P1) namely

$$\hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \leq 2\Delta\hat{x}, \tag{47}$$

hold. Then, $\hat{x}(u)$ is always monotone nondecreasing on $[0,1]$.

(Proof) When (P1) holds, the graph of $\hat{x}^{(1)}(u)$ is concave down or a straight line, yielding $\hat{x}^{(1)}(u) \geq 0 \ \forall u \in [0,1]$ by (46). □

The following Lemma holds for the case (P2).

[**Lemma 2**] Assume that (46) and (P2) namely

$$\hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) > 2\Delta\hat{x}, \tag{48}$$

hold. Then, $\hat{x}(u)$ is monotone nondecreasing on $[0,1]$, if and only if at least one of the following three conditions holds:

$$2\hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \leq 3\Delta\hat{x} \tag{49}$$
$$\hat{x}^{(1)}(0) + 2\hat{x}^{(1)}(1) \leq 3\Delta\hat{x} \tag{50}$$
$$\begin{aligned} &\left(\hat{x}^{(1)}(0) - 2\Delta\hat{x}\right)^2 + \left(\hat{x}^{(1)}(1) - 2\Delta\hat{x}\right)^2 \\ &\quad + \left(\hat{x}^{(1)}(0) - 2\Delta\hat{x}\right)\left(\hat{x}^{(1)}(1) - 2\Delta\hat{x}\right) \leq 3\Delta\hat{x}^2. \end{aligned} \tag{51}$$

(Proof) By (42) and (P2), the function $\hat{x}^{(1)}(u)$ is a concave up parabola, and it has a global minimum at $u^\star \in \mathbf{R}$ given by

$$u^\star = -\frac{q_j}{p_j} = \frac{\hat{x}^{(1)}(1) + 2\hat{x}^{(1)}(0) - 3\Delta\hat{x}}{3(\hat{x}^{(1)}(1) + \hat{x}^{(1)}(0) - 2\Delta\hat{x})}. \tag{52}$$

Then, under the assumption (46), we see that $\hat{x}^{(1)}(u) \geq 0 \ \forall u \in [0,1]$ if and only if one of the three conditions (i), (ii) and (iii) holds, where (i) $u^\star \le 0$, (ii) $u^\star \ge 1$ and (iii) $0 < u^\star < 1$ with $\hat{x}^{(1)}(u^\star) \ge 0$. Using (52) and noting (48), the first two cases (i) and (ii) are written as the conditions (49) and (50) respectively. On the other hand, the condition $\hat{x}^{(1)}(u^\star) \ge 0$ in (iii) is written as

$$\begin{aligned}\hat{x}^{(1)}(u^\star) &= \frac{1}{2}\left(p_j\left(-\frac{q_j}{p_j}\right)^2 + 2q_j\left(-\frac{q_j}{p_j}\right) + r_j\right)\\ &= \hat{x}^{(1)}(0) - \frac{\left(\hat{x}^{(1)}(1) + 2\hat{x}^{(1)}(0) - 3\Delta\hat{x}\right)^2}{3\left(\hat{x}^{(1)}(1) + \hat{x}^{(1)}(0) - 2\Delta\hat{x}\right)}\\ &\ge 0, \end{aligned} \tag{53}$$

which can be rewritten as the condition (51). The proof is completed by noting that the restriction $0 < u^\star < 1$ in (iii) is ignored in the assertion of this lemma, and instead the phrase 'at least' is included. □

Now we summarize the results in Lemmas 1 and 2 as a theorem. For this purpose, each condition is illustrated as a region in $(\hat{x}^{(1)}(0), \hat{x}^{(1)}(1))$-coordinate plane in Figure 1. Assuming (46) with $\Delta\hat{x} > 0$ in all the cases, the condition (47) is shown by a triangular region (R1), the conditions (49) and (50) with (48) by triangular regions (R2) and (R3) respectively, and (51) by the ellipse (R4).

Then, we see that the necessary and sufficient condition for $\hat{x}(u)$ to be monotone nondecreasing on $[0,1]$ is that $(\hat{x}^{(1)}(0), \hat{x}^{(1)}(1))$ belongs to the union of (R1)-(R4), i.e. the fan-shaped region in Figure 1 bounded by the outer curve of the ellipse in (R4), $\hat{x}^{(1)}(0)$-, and $\hat{x}^{(1)}(1)$-axes. Noting that the region (R4) can be rewritten as

$$\begin{aligned}&3\Delta\hat{x} - \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)}\\ &\le \hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \le 3\Delta\hat{x} + \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)},\end{aligned} \tag{54}$$

the fan-shaped region is separated into disjoint sets and we obtain the following condition.

[**Theorem 1**] The curve $\hat{x}(u)$ is monotone nondecreasing on $[0,1]$, if and only if the following condition Ω holds:

$$\Omega: \begin{cases} \hat{x}^{(1)}(0) \ge 0, \quad \hat{x}^{(1)}(1) \ge 0, \quad \Delta\hat{x} \ge 0 \quad \text{and} \\ \hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \le 3\Delta\hat{x} + \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)} \\ \qquad\qquad \text{if } 0 \le \hat{x}^{(1)}(1) \le 3\Delta\hat{x} \\ 3\Delta\hat{x} - \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)} \le \hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \\ \qquad \le 3\Delta\hat{x} + \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)} \\ \qquad\qquad \text{if } 3\Delta\hat{x} \le \hat{x}^{(1)}(1) \le 4\Delta\hat{x}. \end{cases} \tag{55}$$

Note that, in the case of $0 \le \hat{x}^{(1)}(1) \le 3\Delta\hat{x}$, only the upper curve of the ellipse is used to include the other regions (R1)-(R3).

The above condition Ω in (55) is expressed in terms of the control points τ_i, or its difference $\Delta\tau_i$ defined by

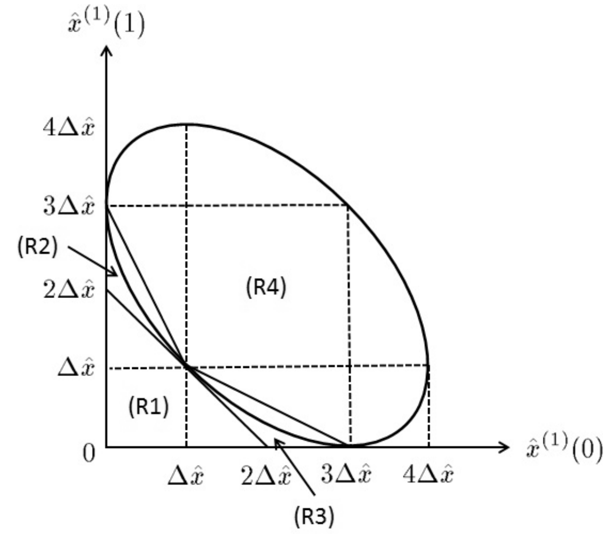

Fig. 1 Regions for monotonicity. R1-R3: triangular regions, R4: elliptic region

$$\Delta\tau_i = \tau_i - \tau_{i-1}. \tag{56}$$

Using (37), (42) and (45), the variables $\hat{x}^{(1)}(0)$, $\hat{x}^{(1)}(1)$ and $\Delta\hat{x}$ are expressed as

$$\hat{x}^{(1)}(0) = \frac{1}{2}(\Delta\tau_{j-1} + \Delta\tau_{j-2}) \tag{57}$$

$$\hat{x}^{(1)}(1) = \frac{1}{2}(\Delta\tau_j + \Delta\tau_{j-1}) \tag{58}$$

$$\Delta\hat{x} = \frac{1}{6}(\Delta\tau_j + 4\Delta\tau_{j-1} + \Delta\tau_{j-2}), \tag{59}$$

hence we have

$$\Omega: \begin{cases} \Delta\tau_{j-1} + \Delta\tau_{j-2} \ge 0, \ \Delta\tau_j + \Delta\tau_{j-1} \ge 0, \\ \Delta\tau_j + 4\Delta\tau_{j-1} + \Delta\tau_{j-2} \ge 0 \quad \text{and} \\ 2\Delta\tau_{j-1} \le \sqrt{(\Delta\tau_j + \Delta\tau_{j-1})(\Delta\tau_{j-1} + \Delta\tau_{j-2})} \\ \qquad\qquad \text{if } 0 \le \hat{x}^{(1)}(1) \le 3\Delta\hat{x} \\ -\sqrt{(\Delta\tau_j + \Delta\tau_{j-1})(\Delta\tau_{j-1} + \Delta\tau_{j-2})} \le 2\Delta\tau_{j-1} \\ \le \sqrt{(\Delta\tau_j + \Delta\tau_{j-1})(\Delta\tau_{j-1} + \Delta\tau_{j-2})} \\ \qquad\qquad \text{if } 3\Delta\hat{x} \le \hat{x}^{(1)}(1) \le 4\Delta\hat{x}. \end{cases} \tag{60}$$

4.2 Monotone Smoothing Splines

We see that the condition Ω in (60) becomes nonlinear in terms of τ in (8), and it may be too complex for practical uses. Thus we present how such results are incorporated in the optimal smoothing spline problems.

Geometric observation in Figure 1 yields a sufficient condition Ω' for monotonic constraint in (31) as

$$\Omega': \begin{cases} 0 \le \hat{x}^{(1)}(0) \le 3\Delta\hat{x} \\ 0 \le \hat{x}^{(1)}(1) \le 3\Delta\hat{x} \end{cases}, \tag{61}$$

which corresponds to the largest square region inscribed within Ω in (60). Then, by (57)-(59), the condition Ω' is rewritten in terms of $\Delta\tau_i$ as

$$\Omega' : \begin{cases} \Delta\tau_{j-1} + \Delta\tau_{j-2} \geq 0 \\ 3\Delta\tau_{j-1} + \Delta\tau_{j-2} \geq 0 \\ \Delta\tau_j + \Delta\tau_{j-1} \geq 0 \\ \Delta\tau_j + 3\Delta\tau_{j-1} \geq 0 \end{cases}, \tag{62}$$

and thus, in terms of the control point τ_i as

$$\Omega' : F\tau_{(j)} \geq 0, \tag{63}$$

where $\tau_{(j)} = [\tau_{j-3}\ \tau_{j-2}\ \tau_{j-1}\ \tau_j]^T$ and

$$F = \begin{bmatrix} -1 & 0 & 1 & 0 \\ -1 & -2 & 3 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & -3 & 2 & 1 \end{bmatrix}. \tag{64}$$

Hence, the monotonic constraint in (31) can be expressed as a linear constraint on the control point vector τ in (8) as

$$H_j\tau \geq 0, \tag{65}$$

where the matrix $H_j \in \mathbf{R}^{4\times M}$ is given by

$$H_j = \left[\, 0_j\ \ F\ \ 0_{M-(j+4)} \,\right]. \tag{66}$$

We note that the condition obtained in [17] corresponds to

$$\bar{\Omega} : \begin{cases} \Delta\tau_{j-2} \geq 0 \\ \Delta\tau_{j-1} \geq 0 \\ \Delta\tau_j \geq 0 \end{cases} \tag{67}$$

and hence it is relaxed to (62) by the present study as we observe in Figure 2, although this is still a sufficient condition, i.e. (62) implies (31) but not vice versa. The condition (62) is meaningful for practical uses, since it is linear in τ_i and the rectangular region in Figure 1 associated with Ω' covers large part of that for Ω in (60).

Also note that the interval in (11) can be easily extended to any knot point interval $[t_j, t_l]$ ($l > j$) including the entire interval $[t_0, t_m]$. Thus, in principle, the monotonicity can be controlled for each knot point interval, e.g. $x(t)$, $t \in [t_0, t_m]$ is monotone nondecreasing on $[t_j, t_l]$ and nonincreasing on $[t_{j'}, t_{l'}]$, where (65) is to be understood like $(-H_j)\tau \geq 0$ for the latter (see Remark 1).

The formulation of **Problem 1** becomes very simple and is very well fit for numerical solutions as convex quadratic programing (QP) problems. Namely, the optimal smoothing splines are obtained by minimizing the convex quadratic cost $J(\tau)$ as shown in (14), whereas monotonic constraints is expressed as linear constraints on τ. A general form of problems becomes as follows:

$$\min_{\tau \in \mathbf{R}^M} J(\tau) = \frac{1}{2}\tau^T G\tau + g^T\tau \tag{68}$$

subject to the constraints of the form

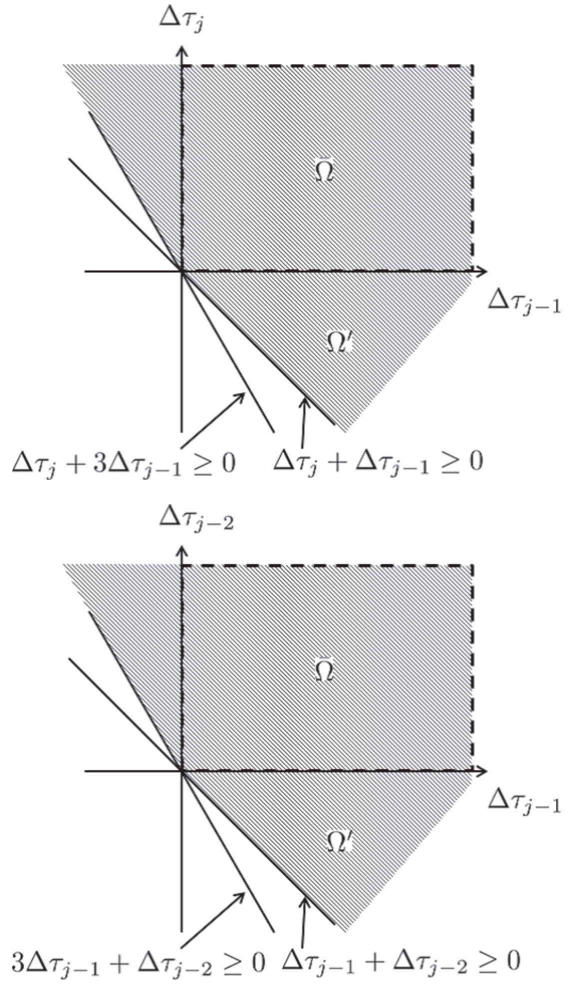

Fig. 2 Monotonic conditions Ω' and $\bar{\Omega}$ on o-$\tau_{j-1}\tau_j$ (top) and o-$\tau_{j-1}\tau_{j-2}$ (bottom) planes

$$H\tau \geq 0, \tag{69}$$

for appropriate matrix H. This problem can be readily solved by various numerical computation methods (see [22] for details). Here we use the function "quadprog" in MATLAB Optimization Toolbox.

(Remark 3) In the present case of cubic splines, convexity constraint on $x(t)$ such as

$$x^{(2)}(t) \geq 0, \quad \forall t \in [t_j, t_{j+1}] \tag{70}$$

can be imposed as a necessary and sufficient condition on τ_i, since $x^{(2)}(t)$ on $[t_j, t_{j+1}]$ is linear in t. Specifically, (70) holds if and only if the pointwise conditions $x^{(2)}(t_j) \geq 0$ and $x^{(2)}(t_{j+1}) \geq 0$ hold, which are expressed respectively as

$$\Delta\tau_{j-1} - \Delta\tau_{j-2} \geq 0, \quad \Delta\tau_j - \Delta\tau_{j-1} \geq 0 \tag{71}$$

by using (35), (43), (41) and (57)-(57). As before, this condition can be expressed in the form of $H_j'\tau \geq 0$, and can be included in addition to the monotonicity constraint (65) for (31) if necessary.

(Remark 4) For an optimal estimation of the smoothing parameter λ, we use the so-called ordinary cross validation method (see e.g.[1]) as follows: Let $\mathcal{D}_l$ be the data set obtained from $\mathcal{D}$ in (7) by deleting the l-th data, i.e.

$$\mathcal{D}_l = \mathcal{D} - \{(u_l, d_l)\},\ l = 1,2,\cdots,N, \tag{72}$$

and let $x^\star_{\lambda,l}$ be the spline constituted from the solution of the above QP problem for the data $\mathcal{D}_l$. Then an optimal $\lambda^\star$ is estimated by minimizing the cross validation function $V(\lambda)$,

$$V(\lambda) = \sum_{l=1}^{N} w_l \left(x^\star_{\lambda,l} - d_l\right)^2. \tag{73}$$

5. Numerical Studies

We examine the design method presented in the previous sections numerically. Specifically, we design the splines $x(t)$ in the time interval $[t_0, t_m] = [0,10]$ by imposing the monotonic constraints

$$x^{(1)}(t) \geq 0,\ \forall t \in [0,10]. \tag{74}$$

The data d_i in (2) is obtained by sampling the function $f(t)$,

$$f(t) = \frac{1}{1 + e^{-0.5(t + \sin t)}}. \tag{75}$$

The number of data is set as $N = 50$, the data points s_i's are randomly spaced in the interval $[t_0, t_m] = [0,10]$, and the magnitude of the additive Gaussian noise in d_i is set as $\sigma = 0.05$. The design parameters w_i and α are set as $w_i = \dfrac{1}{N}$ and $\alpha = 1$ respectively. The optimal weight τ is obtained by the method in Section **4.2** and (62) for the constraints in (74), and then we compute $x(t)$ by (1).

Figure 3 shows the result of $x(t)$ in solid lines, where the data points (s_i, d_i) are shown by asterisk $*$. For the sake of comparison, we plotted the results for the smoothing spline $x_p(t)$ based on the monotonic condition in [17], i.e. (67), and the unconstrained spline $x_0(t)$ without imposing any constraints. In Figure 4, the corresponding values of cross validation function $V(\lambda)$ in (73) are plotted in the interval $[10^{-7}, 10]$. The optimal value of smoothing parameter λ was estimated as $\lambda^\star = 3.9811 \times 10^{-4}$ for all the cases, whereas the values of $V(\lambda^\star)$ differ from each other as shown in Table 2. The function $f(t)$ is plotted in dashed lines. Also, the corresponding first derivative $x^{(1)}(t)$ and $\Delta\tau_j$, $j = -2, -1, \cdots, 9$ are plotted in Figures 5 and 6 respectively. From these results, we conclude that the monotonic spline $x(t)$ results in satisfactory approximation of original function $f(t)$ while preserving the monotone nondecreasing property specified as (74), which is not the case with $x_0(t)$. Moreover, we see from Figure 6 that the monotonicity condition derived here relaxes the one developed in [17].

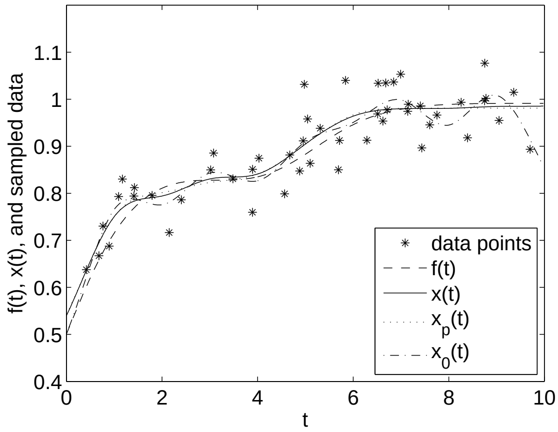

Fig. 3 Design example of monotone smoothing spline $x(t)$ versus monotone smoothing spline $x_p(t)$ in **[9]** and unconstrained spline $x_0(t)$

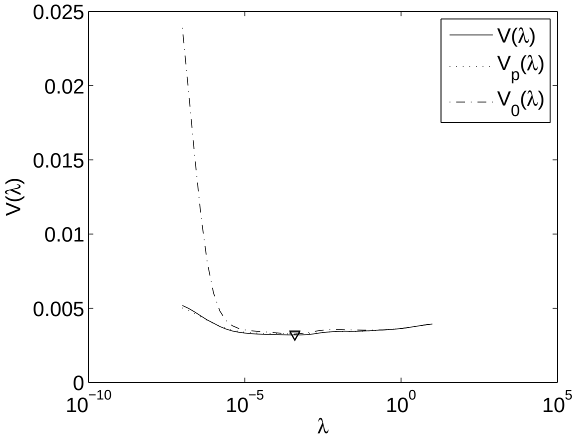

Fig. 4 Cross validation function $V(\lambda)$

Table 2 Values of $V(\lambda^\star)$, $V_p(\lambda^\star)$ and $V_0(\lambda^\star)$ at $\lambda^\star = 3.9811 \times 10^{-4}$

$V(\lambda^\star)$	3.1983×10^{-3}
$V_p(\lambda^\star)$	3.2749×10^{-3}
$V_0(\lambda^\star)$	3.2601×10^{-3}

6. Concluding Remarks

In this paper, we developed a method for designing optimal monotone smoothing splines for the cubic case. We employed B-spline approach and hence the central issue is to determine an optimal control point vector τ. We derived a condition for monotonic spline over interval based on the results of Fritsch and Carlon's works in [18]. In particular, it is derived as a necessary and sufficient condition on control points, and then we derived a sufficient condition for practical uses, thereby relaxing the sufficient condition developed in [17].

We also presented how these results are incorporated in the optimal smoothing spline problems. As results, the design problem becomes a convex QP problem in τ, where very efficient numerical algorithms are available. We examined the performances

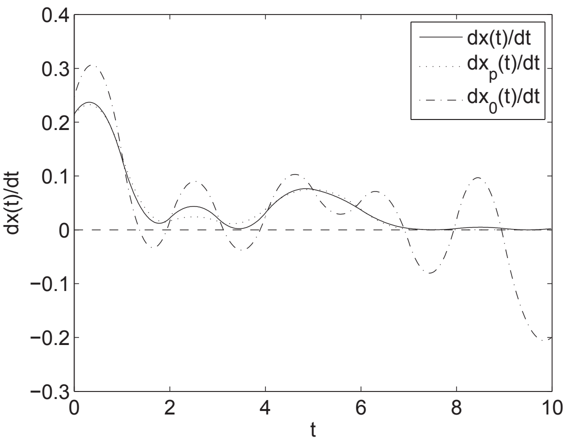

Fig. 5 Corresponding first derivative $x^{(1)}(t)$

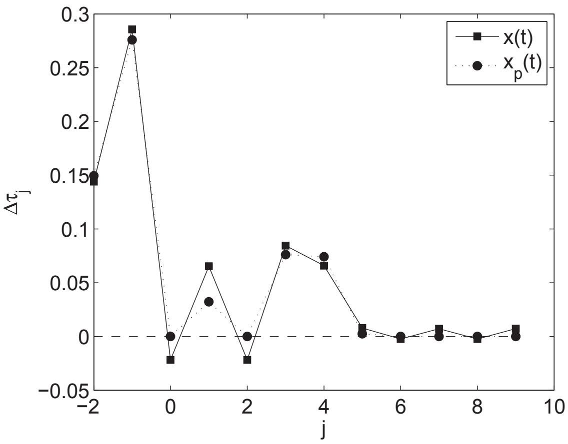

Fig. 6 Corresponding difference of control point $\Delta\tau_j(=\tau_j-\tau_{j-1}),\ j=-2,-1,\cdots,9$

of the design method by numerical example.

Future works naturally include an extension of this result on the cubic case to higher degrees as quartic or quintic splines. However, as the results in [19,20] on quartic or quintic polynomials indicate, the treatments are significantly different from the cubic case and it requires much more detailed studies to obtain practical and efficient algorithms. On the other hand, based on our past works (e.g. [8]), the extensions of this results for one-dimensional case (i.e. curves) to the two-dimensional case (i.e. surfaces) will be straightforward. This also indicates that the same line of the approach using B-splines can be used for extensions to even higher dimensions.

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