Monotone Smoothing Spline Curves Using Normalized Uniform Cubic B-splines

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Abstract
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 along the line of Fritsch and Carlson’s works in \cite{1}. Moreover, we present how these results are incorporated in the optimal smoothing spline problems. The performance is examined by some numerical examples.

1 Introduction

The interpolating and smoothing splines have been developed as basic tools for constructing continuously differentiable curves from a given set of discrete data (see e.g. \cite{2, 3, 4}).

While they are useful in real applications, 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 (see e.g. \cite{5, 6, 7}). Recently, the authors have also considered such problems by employing B-spline approach \cite{8, 9}. Specifically, we have shown that various types of constraints can be formulated as linear constrains 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 cubic case. We employ normalized uniform cubic B-splines as the basis functions. In particular, we derive a condition for monotonic constraints over interval along the line of Fritsch and Carlson’s works in \cite{1}. Our results will be similar to those in \cite{1} for monotone Hermite cubic interpolation, but differ in that we give a condition for the monotonicity as linear function in terms of control points. Although the new condition is again sufficient, we see that it relaxes the one developed in \cite{9}. 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 degrees as quartic or quintic splines are desirable, but they are quite 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 for only the cubic case. We design curves $x(t)$ by employing normalized, uniform cubic B-spline function $B_3(t)$ as the basis functions,

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

(1)

where $m$ is an integer, $\tau_i \in \mathbb{R}$ 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

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

(2)

Then $x(t)$ formed in (1) is a spline of degree 3 with the knot points $t_i$. By an appropriate choice of $\tau_i$’s, arbitrary spline of degree 3 can be designed in the interval $[t_0,t_m]$. 

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Here $B_3(t)$ is defined by

$$B_3(t) = \begin{cases} 
    N_{3-j,3}(t-j) & j \leq t < j+1, \\
    0 & j = 0,1,2,3. 
\end{cases} \quad (3)$$

The basis elements $N_{j,3}(t)$ ($j = 0,1,2,3$), $0 \leq t \leq 1$ can be obtained recursively by the improved de Boor and Cox's algorithm (see e.g. [10]), and then we have

$$\begin{align*}
N_{0,3}(t) &= \frac{1}{3!}(1-t)^3 \\
N_{1,3}(t) &= \frac{1}{3!}(4-6t+3t^2) \\
N_{2,3}(t) &= \frac{1}{3!}(1+3t+3t^2-3t^3) \\
N_{3,3}(t) &= \frac{1}{3!}t^3. 
\end{align*} \quad (4)$$

Thus, $B_3(t)$ is a piecewise polynomial of degree 3 with integer knot points and is second continuously differentiable. It is noted that $B_3(t)$ is normalized in the sense $\sum_{j=0}^3 N_{j,3}(t) = 1, \quad 0 \leq t \leq 1.$

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

$$x(t) = \sum_{i=-3+j}^j \tau_i B_3(\alpha(t-t_i)), \quad (5)$$

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

$$\mathcal{D} = \{(u_i,d_i): t_i \in [t_0,t_m], \quad d_i \in \mathbb{R}, \quad i = 1,\ldots,N\}, \quad (6)$$

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

$$\tau = \begin{bmatrix} \tau_{-3} & \tau_{-2} & \cdots & \tau_{m-1} \end{bmatrix}^T. \quad (7)$$

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

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

$$\min_{\tau \in \mathbb{R}^m} J(\tau)$$

subject to

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

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

$$J(\tau) = \lambda \int_{t_0}^{t_m} \left( x^{(2)}(t) \right)^2 dt + \sum_{i=1}^N w_i (x(u_i) - d_i)^2, \quad (8)$$

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

**Remark 1** The above inequality ‘$\geq$’ in (8) can be readily replaced with ‘$\leq$’ 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. [10]).

First, in order to express (9) in terms of the vector $\tau$, we introduce $b(t) \in \mathbb{R}^M$ and a matrix $B \in \mathbb{R}^{M \times N}$ defined respectively as

$$b(t) = \begin{bmatrix} B_3(\alpha(t-t_3)) & B_3(\alpha(t-t_2)) & \cdots & B_3(\alpha(t-t_{m-1})) \end{bmatrix}^T, \quad (10)$$

$$B = \begin{bmatrix} b(u_1) & b(u_2) & \cdots & b(u_N) \end{bmatrix}. \quad (11)$$

Then, noting that $x(t)$ is expressed as $x(t) = \tau^T b(t)$, the cost function in (9) is written as

$$J(\tau) = \tau^T G \tau - 2\tau^T g + r \quad (12)$$

with

$$G = \lambda Q + B W B^T \quad (13)$$

$$g = B W d \quad (14)$$

$$r = d^T W d, \quad (15)$$

where

$$W = \text{diag}\{w_1, w_2, \ldots, w_N\} \quad (16)$$

$$d = \begin{bmatrix} d_1 & d_2 & \cdots & d_N \end{bmatrix}^T. \quad (17)$$

Also, $Q \in \mathbb{R}^{M \times M}$ in (13) is a Gramian defined by

$$Q = \int_{t_0}^{t_m} \frac{d^2 b(t)}{dt^2} \frac{d^2 b^T(t)}{dt^2} dt. \quad (18)$$

Once $\alpha$ and $m$ in (1) are set, the Gramian $Q$ is computed explicitly as follows (see e.g. [10]): By introducing a new integration variable $t' = \alpha(t-t_0)$, we have $dt' = \alpha dt$. Moreover, (2) yields $\alpha(t-t_i) = t' - \alpha(t_i - t_0) = t' - i$. Then we find that

$$Q = \alpha^3 R, \quad (19)$$

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

$$R = \int_0^m \hat{b}^{(2)}(t) \hat{b}^{(2)}(t)^T dt, \quad (20)$$

with

$$\hat{b}(t) = \begin{bmatrix} B_3(t-3) & B_3(t-2) & \cdots & B_3(t-(m-1)) \end{bmatrix}^T. \quad (21)$$

Here, it can be shown that $R$ is obtained by

$$R = R_{\infty} - (R_- + R_+), \quad (22)$$

where

$$R_{\infty} = \int_{-\infty}^{+\infty} \hat{b}^{(2)}(t) \hat{b}^{(2)}(t)^T dt.$$
For the optimal smoothing splines \(x(t)\) in the previous section, we next consider to impose the following monotonic condition

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

(27)

Our task here is to express such constraints in terms of the control points \(\tau_i\). In the sequel, we first derive a condition for monotonic constraints over knot interval along the line of Fritsch and Carlson’s work [1] (Section 4.1). Then, we present how such results are incorporated in the optimal smoothing spline problems (Section 4.2).

4 Monotone Smoothing Splines

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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 (5) by (3) as

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

(28)

Thus, we see that \(x(t)\) depends on only the four weights \(\tau_{j-3}, \tau_{j-2}, \tau_{j-1}, \tau_j\). Moreover, by introducing a new variable \(u, \quad u = \alpha(t - t_j), \quad \alpha \geq 0\), the interval \([t_j, t_{j+1}]\) in \(t\) is normalized to \([0, 1]\) in \(u\). We then rewrite \(x(t)\) in (28) as \(x(u)\),

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

(30)

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 (30) by

\[
x^{(l)}(t) = \alpha^l x^{(l)}(u), \quad l = 0, 1, 2, 3,
\]

(31)

with

\[
x^{(l)}(u) = \sum_{i=0}^{3} \tau_{j-3+i} N^{(l)}_{i,3}(u).
\]

(32)

Using (4), we obtain an explicit form for \(x(u)\) in (30) as

\[
x(u) = \frac{1}{6} (p_j u^3 + 3 q_j u^2 + 3 r_j u + s_j)
\]

with

\[
p_j = \tau_j - 3 \tau_{j-1} + 3 \tau_{j-2} - \tau_{j-3}, \quad q_j = \tau_{j-1} - 2 \tau_{j-2} + \tau_{j-3}, \quad r_j = \tau_{j-1} - \tau_{j-3}, \quad s_j = \tau_{j-1} + 4 \tau_{j-2} + \tau_{j-3},
\]

and thus

\[
x^{(1)}(u) = \frac{1}{2} (p_j u^2 + 2 q_j u + r_j).
\]

(33)

Now we consider monotonicity constraints (27) or equivalently \(x^{(1)}(u) \geq 0 \forall u \in [0, 1]\) for \(x(u)\) in (33).

We follow the approach employed in [1], where the constraints are examined using the boundary values of the curve, i.e. \(x(0), x(1)\), \(x^{(1)}(0)\) and \(x^{(1)}(1)\) in the present case. In particular, we find the range of \(x^{(1)}(0)\) and \(x^{(1)}(1)\), in which the condition (27) holds, for each points \(x(0)\) and \(x(1)\). Note that these values can then be rewritten in terms of the four control points \(\tau_{j-3}, \tau_{j-2}, \tau_{j-1}, \tau_j\) using the following relations.

\[
p_j = 6(x^{(1)}(1) + x^{(1)}(0) - 2x^{(1)}(1) + 2x^{(1)}(0))
\]

\[
q_j = 2(-x^{(1)}(1) - 2x^{(1)}(1) + 3x^{(1)}(1) - 3x^{(1)}(0))
\]

\[
r_j = 2x^{(1)}(0)
\]

(39)

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

\[
\Delta \tilde{x} = \tilde{x}(1) - \tilde{x}(0).
\]

(40)

Then, it is obvious that a necessary condition for monotonicity in (27) is given by

\[
x^{(1)}(0) \geq 0, \quad x^{(1)}(1) \geq 0, \quad \Delta \tilde{x} \geq 0.
\]

(41)
In (41), the case of $\Delta \hat{x} = 0$ (i.e. $\hat{x}(0) = \hat{x}(1)$) is trivial since $\hat{x}(u)$ is then monotone on $[0, 1]$, i.e. a constant, if and only if $\hat{x}^{(1)}(0) = \hat{x}^{(1)}(1) = 0$. Thus, in the sequel, we examine the case of $\Delta \hat{x} > 0$, and the results will finally be stated so as to include the case $\Delta \hat{x} = 0$.

Noting that $\hat{x}^{(1)}(t)$ in (38) is quadratic, we consider the following two cases:

(P1) $p_j \leq 0$

(P2) $p_j > 0$

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

**Lemma 1** Assume that (41) holds. Then, $\hat{x}(u)$ is monotone on $[0, 1]$, if $p_j \leq 0$, i.e.

\[
(R1) \quad \hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \leq 2\Delta \hat{x}. \tag{42}
\]

On the other hand, it can be shown that the following Lemma holds for the case (P2).

**Lemma 2** Assume that (41) holds. Then, $\hat{x}(u)$ is monotone on $[0, 1]$, if $p_j > 0$ and one of the following three conditions holds:

(R2) $2\hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \leq 3\Delta \hat{x}$ \tag{43}

(R3) $\hat{x}^{(1)}(0) + 2\hat{x}^{(1)}(1) \leq 3\Delta \hat{x}$ \tag{44}

(R4) \[
\left(\hat{x}^{(1)}(0) - 2\Delta \hat{x}\right)^2 + \left(\hat{x}^{(1)}(1) - 2\Delta \hat{x}\right)^2 + \left(\hat{x}^{(1)}(0) - 2\Delta \hat{x}\right)\left(\hat{x}^{(1)}(1) - 2\Delta \hat{x}\right) \leq 3\Delta \hat{x}^2. \tag{45}
\]

The regions specified by (R1)-(R4) are illustrated as Figure 1. From the above results, we can conclude that the necessary and sufficient condition for preserving the monotonicity of $\hat{x}(u)$ in (27) is given as the fan-shaped region for $\hat{x}^{(1)}(0)$ and $\hat{x}^{(1)}(1)$ bounded by the upper curve of the ellipse, $\hat{x}^{(1)}(0)$- and $\hat{x}^{(1)}(1)$-axes. The results can be summarized as follows.

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

\[
\Omega : \left\{ \begin{array}{l}
\hat{x}^{(1)}(0) \geq 0, \quad \hat{x}^{(1)}(1) \geq 0, \quad \Delta \hat{x} \geq 0 \\
\hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \leq 3\Delta \hat{x} + \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)} \\
\text{if } 0 \leq \hat{x}^{(1)}(1) \leq 3\Delta \hat{x} \\
3\Delta \hat{x} - \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)} \leq \hat{x}^{(1)}(0) + \hat{x}^{(1)}(1) \\
\leq 3\Delta \hat{x} + \sqrt{\hat{x}^{(1)}(0)\hat{x}^{(1)}(1)} \\
\text{if } 3\Delta \hat{x} \leq \hat{x}^{(1)}(1) \leq 4\Delta \hat{x}.
\end{array} \right. \tag{46}
\]

For our purpose, the condition $\Omega$ in (46) is expressed in terms of $\tau_j$ or its difference, as

\[
\Omega : \left\{ \begin{array}{l}
\Delta \tau_{j-1} + \Delta \tau_{j-2} \geq 0, \quad \Delta \tau_j + \Delta \tau_{j-1} \geq 0, \\
\Delta \tau_j + 4\Delta \tau_{j-1} + \Delta \tau_{j-2} \geq 0 \quad \text{and} \\
2\Delta \tau_{j-1} \leq \sqrt{(\Delta \tau_j + \Delta \tau_{j-1})(\Delta \tau_j + \Delta \tau_{j-2})} \\
\text{if } 0 \leq \hat{x}^{(1)}(1) \leq 3\Delta \hat{x} \\
-\sqrt{(\Delta \tau_j + \Delta \tau_{j-1})(\Delta \tau_j + \Delta \tau_{j-2})} \leq 2\Delta \tau_{j-1} \\
\leq \sqrt{(\Delta \tau_j + \Delta \tau_{j-1})(\Delta \tau_j + \Delta \tau_{j-2})} \\
\text{if } 3\Delta \hat{x} \leq \hat{x}^{(1)}(1) \leq 4\Delta \hat{x}
\end{array} \right. \tag{47}
\]

with

\[
\Delta \tau_j = \tau_j - \tau_{j-1}. \tag{48}
\]

### 4.2 Monotone Smoothing Splines

We see that the condition $\Omega$ in (47) becomes non-linear in terms of $\tau$ in (7), and it may be too complex for practical uses. We here present how such results are incorporated in the optimal smoothing spline problems.

Geometric observation in Figure 1 yields a sufficient condition $\Omega'$ of monotonic constraint in (27) defined as

\[
\Omega' : \left\{ \begin{array}{l}
0 \leq \hat{x}^{(1)}(0) \leq 3\Delta \hat{x} \\
0 \leq \hat{x}^{(1)}(1) \leq 3\Delta \hat{x}
\end{array} \right., \tag{49}
\]

which corresponds to the largest square region inscribed within $\Omega$ in (47). Then, by (34)-(37) and (39), the condition $\Omega'$ is rewritten in terms of $\tau_j$ as

\[
\Omega' : \left\{ \begin{array}{l}
\Delta \tau_{j-1} + \Delta \tau_{j-2} \geq 0 \\
3\Delta \tau_{j-1} + \Delta \tau_{j-2} \geq 0 \\
\Delta \tau_j + \Delta \tau_{j-1} \geq 0 \\
\Delta \tau_j + 3\Delta \tau_{j-1} \geq 0
\end{array} \right. \tag{50}
\]

Hence, the monotonic constraint in (27) can be expressed as a linear constraint in $\tau$, i.e. as

\[
H \tau \geq 0 \tag{51}
\]
optimal smoothing splines are obtained by minimizing the convex quadratic cost $J(\tau)$ as shown in (12), whereas monotonic constraints is expressed as linear constraints on $\tau$. A general form of problems becomes as follows:

$$
\min_{\tau \in \mathbb{R}^d} J(\tau) = \frac{1}{2} \tau^T G \tau + g^T \tau
$$

subject to the constraints of the form

$$
H \tau \geq 0,
$$

for appropriate matrix $H$. This problem can be readily solved by various numerical computation methods (see [11] for details). Here we use the command “quadprog” in MATLAB Optimization Toolbox.

5 Numerical Studies

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

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

For designing optimal smoothing splines $x(t)$, the data $d_i$ in (2) is obtained by sampling the function $f(t)$,

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

The number of data is set as $N = 15$, 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 $\sigma = 0.1$. The design parameters $\lambda$, $w_i$ and $\alpha$ are set as $\lambda = 10^{-3}$, $w_i = \frac{1}{5}$, and $\alpha = 1$ respectively. The optimal weight $\tau$ is obtained by the method in Section 4.2 and (50) for the constraints in (55), and then we compute $x(t)$ by (1).

Figure 3 (a) shows the result of $x(t)$ in solid lines, where the data points $(s_j, d_j)$ 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 [9], i.e. (52), and the unconstrained spline $x_{o}(t)$ without imposing any constraints. 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 Figure 3 (b) and (c) respectively. From these results, we may conclude that the monotonic splines $x(t)$ results in satisfactory approximation of original one $f(t)$ while preserving the monotone nondecreasing property specified as (55), which is not the case with $x_{o}(t)$.

6 Concluding Remarks

In this paper, we developed a method for designing optimal monotone smoothing splines for the cubic case.
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 \( \tau \), where very efficient numerical algorithms are available. We examined the performances of the design method by numerical example.

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**References**


