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Optimal Smoothing Splines for Detecting Extrema from Observational Data

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Abstract— **In this paper, we present a method for detecting and computing the extrema from observational data by using spline curves. First, we approximate a given set of discrete data by designing optimal smoothing spline curves using normalized uniform B-splines as the basis functions. Then, we show the method for detecting and computing all the extrema of designed splines and/or of its first derivative. Here, utilizing the fact that splines are continuously differentiable piecewise polynomials, we only need to detect and compute the extrema of the polynomial and its first derivative in turn for each interval between the knot points. This process is easily carried out since the polynomial in each interval is characterized by a few control points. Finally we verified the validities by numerical experiments. In particular, the detection and computation of the extrema of the first derivative are used for edge detection in digital images.**

I. Introduction

We consider the problem of detecting and computing the extrema from given observational data. Let $f(t)$ be a smooth function defined in an interval $[t_1, t_m]$ and a set of discrete data $(u_i, d_i),\ u_i \in [t_1, t_m],\ d_i \in \mathrm{R},\ i = 1, 2, \cdots, N$ be given, where d_i are assumed to be obtained by sampling $f(t)$ with or without noises. Here, the function $f(t)$ is unknown in general. Then, the problem we consider is to develop a method for estimating all the extrema of $f(t)$ and its first derivative in a systematic fashion. Thus, it enables us to estimate the global maximum and minimum. Obviously, the problem of detecting extrema is one of the main issues in various kinds of optimization problems and mathematical programming, whereas the extrema of the first derivative $f^{(1)}(t)$ (inflection points of $f(t)$) may be used, for instance, for edge detection problem in a digital image data.

A natural approach to this problem would be first to interpolate or approximate the given points by some functions and then to find their extrema. It is recognized, however, that the interpolation often results in an oscillatory curve, and hence inappropriate for our purpose. On the other hand, the approximation by smoothing splines is stable numerically and yields feasible approximation results.

The splines have been used in various fields of engineering such as computer aided design, computer vision, robotics, and image processing, etc. and have been studied extensively (see e.g. [1], [2]). In particular, a fairly recent development of 'dynamic splines' employs optimal control theory and provided a new framework for the theory of splines [3]. Also, such an approach has then been taken for analyzing B-spline functions [4]. On the other hand, using normalized uniform B-splines as the basis functions, the authors developed the method for designing optimal interpolating and smoothing splines [5]. Also we applied the method for generating cursive characters and character strings as seen in Japanese calligraphy [6].

This paper is a continuation of our studies on the optimal design of splines based on B-splines. For our present purpose, we assume that the data are obtained by sampling some function $f(t)$ with or without noises. Then we show that the optimal smoothing spline designed for the sampled data converges to a limiting spline curve as the number of sample points N tends to infinity. This limiting curve is represented as a functional of $f(t)$. Such a convergence property was studied in [7] in a dynamical systems setting, namely for spline curves generated as the output of linear dynamical systems.

Then, for estimating and computing all the extrema of $f(t)$ and its derivative $f^{(1)}(t)$, we can fully utilize the fact that the designed splines are piecewise polynomials and continuously differentiable. Namely we only need to detect and compute the extrema of the polynomial or its derivatives for each interval between the knot points in turn. The detection and computation of the extrema in each interval are carried out using a few control points representing the polynomial. As the result, the global maximum and minimum can be obtained. If the given set of data were not from a smooth function, this method still extracts extremal features hiding behind the data. Such a case arises, for instance, when a digital image is taken from a scene with sharp edges.

This paper is organized as follows: In Section II, we describe the optimal smoothing spline problem. In Section III, the optimal solution is presented, and the asymptotic and statistical properties are analyzed. The algorithms are developed for detecting and computing the extrema of the optimal spline curves in Section IV. The results of numerical experiments are presented in Section V, and the concluding remarks are given in Section VI.

II. Preliminaries

We design curves $x(t)$ by employing normalized, uniform B-spline function $B_k(t)$ of degree k as the basis functions,

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

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

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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 k with the knot points t_i. In particular, by an appropriate choice of τ_i's, arbitrary spline of degree k can be designed in the interval $[t_1, t_m]$.

Here $B_k(t)$ is defined by

$$B_k(t) = \begin{cases} N_{k-j,k}(t-j) & j \le t < j+1,\ j = 0,1,\cdots,k \\ 0 & t < 0 \ \text{ or } \ t \ge k+1, \end{cases} \tag{3}$$

and the basis elements $N_{j,k}(t)$ $(j = 0,1,\cdots,k)$, $0 \le t \le 1$ are obtained recursively by the following algorithm (see e.g. [8]):

Algorithm 1: Let $N_{0,0}(t) \equiv 1$ and, for $i = 1,2,\cdots,k$, compute

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

Thus, $B_k(t)$ is a piece-wise polynomial of degree k with integer knot points and is $k-1$ times continuously differentiable. It is noted that $B_k(t)$ for $k = 0,1,2,\cdots$ is normalized in the following sense $\sum_{j=0}^{k} N_{j,k}(t) = 1,\ 0 \le t \le 1$.

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

$$x(t) = \sum_{i=-k+j}^{j} \tau_i B_k(\alpha(t - t_i)), \tag{5}$$

since, by (3), $B_k(\alpha(t-t_i))$ vanishes in $[t_j, t_{j+1})$ for $i < -k+j$ and $i > j$. Moreover, by (3), we may write

$$x(t) = \sum_{i=0}^{k} \tau_{j-k+i} N_{i,k}(\alpha(t-t_j)), \quad t \in [t_j, t_{j+1}). \tag{6}$$

For the sake of later reference, we list the basis functions $N_{j,k}(t)$ for $k = 3$.

$$\begin{aligned} N_{0,3}(t) &= \frac{1}{3!}(1-t)^3 \\ N_{1,3}(t) &= \frac{1}{3!}(4 - 6t^2 + 3t^3) \\ N_{0,3}(t) &= \frac{1}{3!}(1 + 3t + 3t^2 - 3t^3) \\ N_{0,3}(t) &= \frac{1}{3!}t^3. \end{aligned} \tag{7}$$

Now, suppose that we are given a set of data

$$\mathscr{D} = \{(u_i; d_i) \ : \ t_1 \le u_1 < \cdots < u_N \le t_m, \ d_i \in \mathbf{R},\ i = 1,\cdots,N\}, \tag{8}$$

and let $\tau \in \mathbf{R}^M$ $(M = m+k-1)$ be the weight vector defined by

$$\tau = \left[\ \tau_{-k+1} \quad \tau_{-k+2} \quad \cdots \quad \tau_{m-1} \ \right]^T. \tag{9}$$

Then, as a basic problem for designing optimal smoothing splines, we consider the following problem, where I denotes an interval either $I = (-\infty, +\infty)$ or $I = (t_1, t_m)$.

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

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

where

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

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

III. Optimal Smoothing Spline Curves

In this section, we first present the solution to Problem 1 derived in [5]. Then, we analyze the asymptotical and statistical properties of the solution when the number of samples N tends to infinity and the data contain the noises. Moreover, since cubic splines are most frequently used for practical purposes, we restrict ourselves to the case of $k = 3$.

For the case of $k = 3$, (1) is written as

$$x(t) = \sum_{i=-2}^{m-1} \tau_i B_3(\alpha(t - t_i)). \tag{11}$$

and, with $M = m+2$, $\tau \in \mathbf{R}^M$ in (9) becomes

$$\tau = \left[\ \tau_{-2} \quad \tau_{-1} \quad \cdots \quad \tau_{m-1} \ \right]^T. \tag{12}$$

A. Optimal Solution

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

$$\begin{aligned} b(t) &= \left[\ B_3(\alpha(t-t_{-2})) \quad B_3(\alpha(t-t_{-1})) \quad \cdots \right. \\ & \qquad \left. \cdots \quad B_3(\alpha(t-t_{m-1})) \ \right]^T, \end{aligned} \tag{13}$$

$$B = \left[\ b(u_1) \quad b(u_2) \quad \cdots \quad b(u_N) \ \right]. \tag{14}$$

Then, noting that $x(t)$ is expressed as $x(t) = \tau^T b(t)$, the cost function in (10) is written as

$$J(\tau) = \lambda \tau^T Q \tau + (B^T \tau - d)^T W (B^T \tau - d). \tag{15}$$

Here, $Q \in \mathbf{R}^{M \times M}$ is a Gramian defined by

$$Q = \int_I \frac{d^2 b(t)}{dt^2} \frac{d^2 b^T(t)}{dt^2} dt, \tag{16}$$

and

$$W = \text{diag}\{w_1,\ w_2.\ \cdots,\ w_N\}, \tag{17}$$

$$d = \left[\ d_1 \quad d_2 \quad \cdots \quad d_N \ \right]^T. \tag{18}$$

We then see that optimal weight τ for Problem 1 is obtained as a solution of

$$(\lambda Q + BWB^T)\tau = BWd. \tag{19}$$

Note that this equation has at least one solution, since in general the relation $\text{rank}[S + UU^T, Uv] = \text{rank}[S + UU^T]$ holds for any matrices $S = S^T \ge 0$, U and vector v of compatible dimensions. Obviously, the solution is unique if and only if $\lambda Q + BWB^T > 0$.

Also, the Gramian $Q \in \mathbf{R}^{M\times M}$ in (16) is computed explicitly as follows. By changing the integration variable, we find that

$$Q = \alpha^3 R. \tag{20}$$

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

$$R = \int_{\hat{I}} \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt, \tag{21}$$

where $\hat{I} = (-\infty,+\infty)$ if $I = (-\infty,+\infty)$ and $\hat{I} = (1,m)$ if $I = (t_1,t_m)$, and

$$\hat{b}(t) = [B_3(t-(-2))\ B_3(t-(-1))\ \cdots\ B_3(t-(m-1))]^T. \tag{22}$$

Denoting R for the case of $\hat{I} = (-\infty,+\infty)$ by R_∞, we obtain

$$R_\infty = \frac{1}{6}\begin{bmatrix} 16 & -9 & 0 & 1 & & & & \\ -9 & 16 & -9 & 0 & 1 & & & \\ 0 & -9 & 16 & -9 & 0 & 1 & & \\ 1 & 0 & -9 & 16 & -9 & 0 & 1 & \\ \ddots & & & \ddots & & & \ddots & \\ & \ddots & & & \ddots & & & \\ & & \ddots & & & \ddots & & \\ & & & & 1 & 0 & -9 & 16 \end{bmatrix}, \tag{23}$$

and R_F for the case of $\hat{I} = (1,m)$, is obtained by

$$R_F = R_\infty - (R_- + R_+), \tag{24}$$

where

$$\begin{aligned} R_- &= \int_{-\infty}^{1} \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt \\ &= \frac{1}{6}\left[\begin{array}{ccc|c} 14 & -6 & 0 & \\ -6 & 8 & -3 & 0_{3,M-3} \\ 0 & -3 & 2 & \\ \hline & 0_{M-3,3} & & 0_{M-3,M-3} \end{array}\right], \end{aligned} \tag{25}$$

$$\begin{aligned} R_+ &= \int_{m}^{+\infty} \hat{b}^{(2)}(t)\left(\hat{b}^{(2)}(t)\right)^T dt \\ &= \frac{1}{6}\left[\begin{array}{c|ccc} 0_{M-3,M-3} & & 0_{M-3,3} & \\ \hline & 2 & -3 & 0 \\ 0_{3,M-3} & -3 & 8 & -6 \\ & 0 & -6 & 14 \end{array}\right]. \end{aligned} \tag{26}$$

Remark 1: It can be shown that the matrix Q in (16) is nonsingular if $I = (-\infty,+\infty)$, and singular if $I = (t_1,t_m)$. Thus (19) has a unique solution when $I = (-\infty,+\infty)$. When $I = (t_1,t_m)$, although it depends on the data points $u_i, i = 1,\cdots,N$, there may be infinitely many solutions. In such a case we employ the minimum norm solution, namely the solution τ with minimum Euclidean norm, which is guaranteed to be unique.

B. Asymptotical and Statistical Analyses

Let $f(t)$ be a continuous function in the interval $[t_1,t_m]$. In order to analyze the asymptotic property of the optimal spline curves as the number of data points N increases, we consider the following cost function instead of (10),

$$J_N(\tau) = \lambda \int_I \left(x^{(2)}(t)\right)^2 dt + \frac{1}{N}\sum_{i=1}^{N}(x(u_i) - f(u_i))^2. \tag{27}$$

When the data d_i is obtained by sampling the function $f(t)$ with additive noises

$$d_i = f(u_i) + \varepsilon_i,\ i = 1,2,\cdots,N, \tag{28}$$

we consider a cost function

$$J_N^\varepsilon(\tau) = \lambda \int_I \left(x^{(2)}(t)\right)^2 dt + \frac{1}{N}\sum_{i=1}^{N}(x(u_i) - f(u_i) - \varepsilon_i)^2. \tag{29}$$

We assume that the noises are zero-mean and white, namely $\mathrm{E}\{\varepsilon_i\} = 0$ and $\mathrm{E}\{\varepsilon_i\varepsilon_j\} = \sigma^2\delta_{ij}$ for all i,j. Moreover, for analyzing the asymptotic properties, we introduce a cost function

$$J_c(\tau) = \lambda \int_I \left(x^{(2)}(t)\right)^2 dt + \int_{t_1}^{t_m}(x(t) - f(t))^2 dt. \tag{30}$$

The solutions that minimize the cost functions $J_N(\tau)$, $J_N^\varepsilon(\tau)$ and $J_c(\tau)$ are obtained as follows. The first two cases follow directly from the result in the previous section: The solution τ_N minimizing $J_N(\tau)$ is obtained as a solution of

$$\left(\lambda Q + \frac{1}{N}BB^T\right)\tau = \frac{1}{N}Bf, \tag{31}$$

where Q and B are given in (16) and (14) respectively, and $f = \begin{bmatrix} f(u_1) & f(u_2) & \cdots & f(u_N) \end{bmatrix}^T$. Obviously, τ_N^ε minimizing $J_N^\varepsilon(\tau)$ is a solution of

$$\left(\lambda Q + \frac{1}{N}BB^T\right)\tau = \frac{1}{N}B(f+\varepsilon), \tag{32}$$

where $\varepsilon = \begin{bmatrix} \varepsilon_1 & \varepsilon_2 & \cdots & \varepsilon_N \end{bmatrix}^T$. On the other hand, $J_c(\tau)$ can be written as

$$\begin{aligned} J_c(\tau) &= \tau^T(\lambda Q + R)\tau \\ &\quad -2\tau^T\int_{t_0}^{t_m} b(t)f(t)dt + \int_{t_1}^{t_m} f^2(t)dt, \end{aligned} \tag{33}$$

where

$$R = \int_{t_1}^{t_m} b(t)b^T(t)dt = \frac{1}{\alpha}R_0, \tag{34}$$

$$R_0 = \int_{1}^{m} \hat{b}(t)\hat{b}^T(t)dt. \tag{35}$$

Thus optimal τ denoted by τ_c is obtained as a solution of

$$(\lambda Q + R)\tau = \int_{t_1}^{t_m} b(t)f(t)dt. \tag{36}$$

It can be shown that $R_0 = R_0^T > 0$, hence the optimal τ_c exists and is unique. Moreover, R_0 can be obtained explicitly as in the case of R_F in (24).

Convergence properties are established under the following assumption.

Assumption 1: The sample points $u_i,\ i = 1,2,\cdots,N$, are such that

$$\lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N} g(u_i) = \int_{t_1}^{t_m} g(t)dt \tag{37}$$

for every continuous function $g(t)$ in $[t_1,t_m]$, i.e. they define a convergent quadrature method.

Then, for the case $I = (-\infty,+\infty)$, we can show that the following results hold.

Theorem 1: Assume that the condition (37) holds. Then,

(i) The optimal solutions τ_N, τ_N^ε and τ_c exist uniquely.

(ii) τ_N converges to τ_c as $N \to \infty$.

(iii) $\mathrm{E}\{\tau_N^\varepsilon\} = \tau_N$ and τ_N^ε converges to τ_c as $N \to \infty$ in mean squares sense.

Remark 2: When $I = (t_1, t_m)$, the matrix Q is singular. Thus it is possible that the coefficient matrix $\lambda Q + \frac{1}{N} BB^T$ in (31) and (32) becomes singular depending on the matrix B, i.e. on the data points $u_i, i = 1, \cdots, N$. In such a case, it can be shown that the above theorem still holds with the understanding that we take minimum norm solutions.

IV. Extrema of the Spline and Its First Derivative

In this section, we develop algorithms for computing all the extrema of the spline curve $x(t)$ and its first derivative $x^{(1)}(t)$. The algorithms used together with the optimal smoothing spline design enables us to find extrema in discrete observation data or edges in digital images.

A. Extrema of Smoothing Splines

We first show the method for detecting the extrema of spline curves $x(t)$. Specifically, we find the points $t \in (t_1, t_m)$ satisfying $x^{(1)}(t) = 0$ and $x^{(2)}(t) > 0$ or $x^{(2)}(t) < 0$. Note that we are considering local minima or maxima only in the strict sense.

Since the curve $x(t)$ is a piece-wise polynomial, we examine and find the extrema of the polynomial in each interval $[t_j, t_{j+1})$ for $j = 1, 2, \cdots, m-1$. For simplicity, we consider the case where $k = 3$ in the sequel. Then, by (6), $x(t)$ for the interval $[t_j, t_{j+1})$ is written as

$$x(t) = \sum_{i=0}^{3} \tau_{j-3+i} N_{i,3}(\alpha(t - t_j)), \quad t \in [t_j, t_{j+1}), \tag{38}$$

and it depends on only the four weight coefficients $\tau_{j-3}, \tau_{j-2}, \tau_{j-1}, \tau_j$ given by the method in the previous section. Moreover, by introducing a new variable $\delta = \alpha(t - t_j)$, we may write $x(t)$ in the interval $[t_j, t_{j+1})$ as $\hat{x}(\delta)$,

$$\hat{x}(\delta) = \sum_{i=0}^{3} \tau_{j-3+i} N_{i,3}(\delta), \quad \delta \in [0,1). \tag{39}$$

By (7), we obtain $x(t)$ as

$$\hat{x}(\delta) = \frac{1}{6}\left(p_j \delta^3 + 3q_j \delta^2 + 3r_j \delta + s_j\right), \quad \delta \in [0,1), \tag{40}$$

where p_j, q_j, r_j, and s_j are defined by

$$\begin{aligned} p_j &= \tau_j - 3\tau_{j-1} + 3\tau_{j-2} - \tau_{j-3}, & (41)\\ q_j &= \tau_{j-1} - 2\tau_{j-2} + \tau_{j-3}, & (42)\\ r_j &= \tau_{j-1} - \tau_{j-3}, & (43)\\ s_j &= \tau_{j-1} + 4\tau_{j-2} + \tau_{j-3}. & (44) \end{aligned}$$

Noting that the derivatives of $x(t)$ and $\hat{x}(\delta)$ are related by $x^{(i)}(t) = \alpha^i \hat{x}^{(i)}(\delta)$, $i = 1, 2, 3$ and $\alpha > 0$, the extrema of $x(t)$ in $[t_j, t_{j+1})$ are simply those of $\hat{x}(\delta)$ in $[0,1)$. If we find that $\hat{x}(\delta)$ has an extremum at $\delta = \delta_e \in [0,1)$, then $x(t)$ has the extremum at $t_e = t_j + \frac{1}{\alpha}\delta_e \in [t_j, t_{j+1})$ and the value is given by $x(t_e) = \hat{x}(\delta_e)$.

From (40), we obtain $\hat{x}^{(1)}(\delta)$ as

$$\hat{x}^{(1)}(\delta) = \frac{1}{2}\left(p_j \delta^2 + 2q_j \delta + r_j\right), \quad \delta \in [0,1), \tag{45}$$

Thus, in order to find the extrema, we only need to examine if the following quadratic functions

$$h(\delta) = p_j \delta^2 + 2q_j \delta + r_j, \tag{46}$$

has a root $\delta = \delta_e$ in $[0,1)$ and examine the sign of $h^{(1)}(\delta_e)$. For the case $p_j \neq 0$, we denote the two roots as

$$\delta_+ = \frac{-q_j + \sqrt{q_j^2 - p_j r_j}}{p_j}, \quad \delta_- = \frac{-q_j - \sqrt{q_j^2 - p_j r_j}}{p_j}. \tag{47}$$

This process can be examined in more details if we introduce the following assumption.

Assumption 2: The number of extrema of $x(t)$ in an interval $[t_j, t_{j+1})$ is at most one for each $j = 1, 2, \cdots, m-1$.

Note that, although it is possible for $x(t)$ to possess up to two extrema in $[t_j, t_{j+1})$, we may employ this assumption since such a case is highly unlikely due to the smoothness properties of the optimal curves.

Then, Assumption 2 corresponds to that $\hat{x}(\delta)$ has at most one extremum in the interval $[0,1)$, and the process of examining the existence of extremum can be simplified. Namely, the existence can be judged based on the signs of $\hat{x}^{(1)}(0)$ and $\hat{x}^{(1)}(1)$ as follows. First note that $\hat{x}(\delta)$ in $[0,1)$ is a polynomial of degree at most three, and that the relations $\hat{x}^{(1)}(0) = r_j/2$ and $\hat{x}^{(1)}(1) = r_{j+1}/2$ hold. Then, geometric observations yield the following three cases:

(P1) If $r_j \cdot r_{j+1} < 0$, an extremum exists in $[0,1)$.

(P2) If $r_j \cdot r_{j+1} = 0$, an extremum exists in $[0,1)$ under some additional conditions.

(P3) If $r_j \cdot r_{j+1} > 0$, no extremum exists in $[0,1)$.

For the cases (P1) and (P2), we can establish the following results (Proofs omitted).

Proposition 1: Assume that $r_j \cdot r_{j+1} < 0$. Then, if $r_j > 0$ and $r_{j+1} < 0$, the function $\hat{x}(\delta)$ has a local maximum at $\delta = \delta_e \in (0,1)$, where

$$\delta_e = \begin{cases} \delta_- & \text{if} \quad p_j \neq 0 \\ -\frac{r_j}{2q_j} & \text{if} \quad p_j = 0 \end{cases}. \tag{48}$$

On the other hand, if $r_j < 0$ and $r_{j+1} > 0$, $\hat{x}(\delta)$ has a local minimum at $\delta = \delta_e \in (0,1)$, where

$$\delta = \begin{cases} \delta_+ & \text{if} \quad p_j \neq 0 \\ -\frac{r_j}{2q_j} & \text{if} \quad p_j = 0 \end{cases}. \tag{49}$$

Proposition 2: Assuming that $r_j \cdot r_{j+1} = 0$, the following two cases arise.

(i) The case $r_j = 0$: If $q_j < 0$ (resp., $q_j > 0$), then $\hat{x}(\delta)$ has a local maximum (resp., minimum) at $\delta = \delta_e = \frac{r_j}{p_j} \in (0,1)$, and if $r_j \cdot q_{j+1} \leq 0$, no extremum exists.

(ii) The case $r_j \neq 0$ and $r_{j+1} = 0$: If $r_j > 0$ and $q_{j+1} > 0$ (resp., $r_j < 0$ and $q_{j+1} < 0$), then $\hat{x}(\delta)$ has a local maximum (resp., minimum) at $\delta = \delta_e = \frac{r_j}{p_j} \in (0,1)$, and if $r_j \cdot q_{j+1} \leq 0$, no extremum exists.

Remark 3: It can be shown that $\delta = \frac{r_j}{p_j}$ in Proposition 2 (ii) actually is $\delta_e = \delta_-$ if $q_{j+1} > 0$ and $\delta_e = \delta_+$ if $q_{j+1} < 0$.

The above arguments for detecting and computing the extrema of $x(t)$ are summarized as follows: Given the weights $\tau_{-2}, \tau_{-1}, \cdots, \tau_{m-1}$, compute r_j and r_{j+1} for $j = 1, 2, \cdots, m-1$, and use Propositions 1 and 2 for the case $r_j \cdot r_{j+1} < 0$ and $r_j \cdot r_{j+1} = 0$, respectively. If we find an extremum of $\hat{x}(\delta)$ at $\delta = \delta_e$, then $x(t)$ has the extremum at $t = t_j + \frac{1}{\alpha}\delta_e$.

B. Extrema of the First Derivative of Smoothing Splines

For $x(t)$ in (38), we find the points $t \in (t_1, t_m)$ satisfying $x^{(2)}(t) = 0$ and $x^{(3)}(t) > 0$ or $x^{(3)}(t) < 0$.

The problem is simply to find the extrema of the quadratic function $\hat{x}^{(1)}(\delta)$ in (45) for each interval $[t_j, t_{j+1})$ for $j = 1, 2, \cdots, m-1$.

First notice that the number of extrema in the interval $[0,1)$ is at most one. Also we see that no extrema exists when $p_j = 0$, since in which case $\hat{x}^{(2)}(\delta) = q_j =$ const. and $x^{(3)}(\delta) = 0$. Since $\hat{x}^{(3)}(\delta) = p_j$, we require $p_j \neq 0$ for the existence of an extremum. In this case, $\hat{x}^{(2)}(\delta) = 0$ yields $\delta = -\frac{q_j}{p_j}$. Thus we get the following results.

Proposition 3: An extremum of $x^{(1)}(t)$ exists in the interval $[t_j, t_{j+1})$ if and only if $p_j \neq 0$ and $0 \leq \delta_e < 1$ hold, where $\delta_e = -\frac{q_j}{p_j}$. When it exists, the extremum is obtained at $t = t_j + \frac{1}{\alpha}\delta_e$. Moreover, $p_j > 0$ and $p_j < 0$ imply a local minimum and maximum respectively, and the value is given by

$$x^{(1)}(t_j + \frac{1}{\alpha}\delta_e) = \hat{x}^{(1)}(\delta_e) = \frac{1}{2}\left(-\frac{q_j^2}{p_j} + r_j\right). \qquad (50)$$

V. Numerical Experiments

We examine the performances of detecting the extrema from a given set of data (u_i, d_i), $i = 1, 2, \cdots, N$, in (8), first by using an example function, and then by applying the method to edge detection in a real digital image.

A. Numerical Example

Let us consider the function $f(t)$

$$f(t) = e^{a(t-1)} \cos(b(t-1)) + 1$$

with $a = \frac{1}{m-1} \log \frac{1}{4}$, $b = \frac{2\pi \times 3}{m-1}$ and $m = 50$. We then generate the data (u_i, d_i), $i = 1, 2, \cdots, N$ by sampling this function with noise as in (28). The number of data is set as $N = 30$, u_i's are randomly spaced in the interval $[t_1, t_m] = (1, 50)$, and the magnitude of the additive noise in d_i is set as $\sigma = 0.02$.

By the method in Section III-B with the design parameters $\alpha = 1$ and $I = (t_1, t_m) = (1, 50)$, the optimal weights τ_N^ε and τ_c are computed. Here, we employed the so-called cross-validation method [2] for estimating the smoothing parameter λ, and the optimal value is obtained as $\lambda^\star = 0.1585$. Fig.1 shows the corresponding smoothing curves $x_N^\varepsilon(t)$ (blue line) and $x_c(t)$ (red line) together with the data points (asterisks)

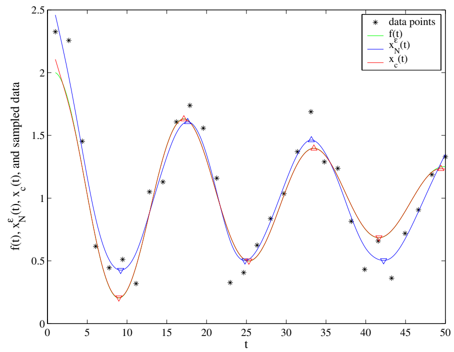


Fig. 1. Optimal smoothing spline curves and their extrema.

and the original curve $f(t)$ (green line). Note that the curves $x_c(t)$ and $f(t)$ are almost indistinguishable.

Using the method described in Section IV-A, we detected and computed the extrema of the designed curves as shown in Fig.1. Here, the triangle and inverted triangle marks respectively denote local maxima and minima, and the same colors are used as for the respective curves. Although the number of the data is relatively small (i.e. $N = 30$) and the data contain noises, we observe that all the extrema of the original curve $f(t)$ are detected fairly precisely. Thus we obtain the global maximum and minimum. Moreover, as the number of data N increases, they are guaranteed to converge to those of $x_c(t)$ which is almost the same as the original curve $f(t)$, implying that the extrema of $f(t)$ can be found almost perfectly.

Note that this convergence properties do not require the exact information on the original curve $f(t)$. Namely, this method works if we know that the the data (u_i, d_i), $i = 1, 2, \cdots, N$ are the samples from some (unknown) function, and that the sample points u_i satisfy Assumption 1.

B. Edge Detection

Suppose that we are given the digital image data $f(i,j)$, $i = 1, 2, \cdots, n$, $j = 1, 2, \cdots, m$, with $f(i,j)$ denoting the gray level of the ij-th pixel. Then we can use the method in Section IV-B for detecting the extrema of the first derivative of smoothing spline curves for the edge detection problem. Since we are considering curves and not surfaces in this paper, the two-dimensional data $f(i,j)$ is processed row by row. Namely, letting the data (u_i, d_i) be the l-th row as $u_i = i$, $d_i = f(l, i)$, $i = 1, 2, \cdots, m$, we first design the optimal spline curve $x(t)$. Then we find the extremal points $t \in (1, m)$ of its first derivative and detect the edges.

The extremal points, however, do not necessarily correspond to the real edges. Figure 2 shows the optimal smoothing spline and its derivatives for the data sampled from a step function. We observe that the 'phantom edges' (two circled extrema) as pointed out in [9] are detected at the double step of the step function. Thus we follow the development in [9] to detect the 'authentic edge' as the extremal point t such that

$$\frac{dx(t)}{dt}\frac{d^3x(t)}{dt^3} < 0. \qquad (51)$$

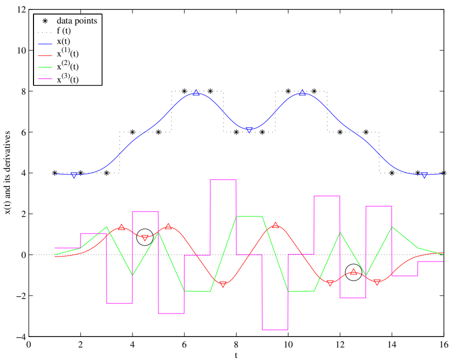


Fig. 2. Optimal smoothing spline and its derivatives for step function.

In addition, in order to suppress the smaller edge contrast, we introduce a threshold value ρ (>0). Namely, we detect the edges as the extremal point t of $x^{(1)}(t)$ satisfying (51) and $|x^{(1)}(t)| > \rho$.

Figure 3 shows the results of edge detection, where (a) is the original image of size 256×256 [pixel] and (b) is the result by the present method with $\lambda = 0.03$ and $\rho = 5$. For the sake of comparison, the results by the sobel and canny edge detection methods are shown in (c) and (d) respectively. Also we tested the performances for noisy data, and the results are shown in Figure 4. In this case, the noisy image in (a) is generated from the image in Figure 3 (a) by adding Gaussian white noise with zero mean and 0.01 variance. The parameters used for Figure 4 (b) are $\lambda = 0.03$ and $\rho = 10$. We may observe that, although the horizontal edges can not be detected by this one-dimensional treatment, the present method works quite well even in the presence of noises. It should be noted that Figure 4 (c) and (d) are obtained by applying each operator directly to the noisy image in (a), i.e. without any pre-processings on (a).

VI. Concluding Remarks

We presented the method for detecting and computing the extrema from observational data by using spline curves. The given data are approximated by optimal smoothing splines using normalized uniform B-splines as the basis functions. The expression for the optimal spline is concise as well as suitable numerical computations. For the data obtained by sampling a function $f(t)$ with or without noises, we showed that the optimal splines $x(t)$ converge to a limiting spline $x_c(t)$ as the number of samples tends to infinity. All the extrema of the optimal spline $x(t)$ and its first derivative can then be found, where the fact that the splines are continuously differentiable piecewise polynomials is fully utilized. If the function $f(t)$ is available, then we can compute the limiting spline $x_c(t)$ and find all its extrema as the approximations to those of $f(t)$. The validities are confirmed by a numerical example and by detecting edges in digital images. Actually, the latter case should be treated in two dimensions, namely via surface design and its extrema computation, and this problem is under study.

(a) original image

(b) proposed method

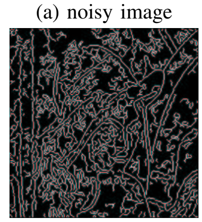
(c) canny filter

(d) sobel filter

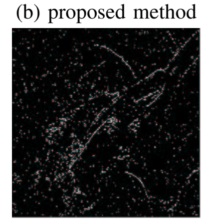
Fig. 3. Results of edge detection for an original image.

(a) noisy image

(b) proposed method



(c) canny filter



(d) sobel filter

Fig. 4. Results of edge detection for a noisy image.

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