Abstract: We consider a problem of designing optimal smoothing spline curves using normalized uniform B-splines as basis functions. Assuming that the data for smoothing is obtained by sampling some curve with noises, an expression for optimal curves is derived when the number of data becomes infinity. It is then shown that, under certain condition, optimal smoothing splines converge to this curve as the number of data increases. The design method and analyses are extended to the case of periodic splines. Results of numerical experiments for periodic case are included for contour synthesizing problem.

Keywords: B-splines, smoothing splines, periodic splines, contour synthesis

1. INTRODUCTION

As is well-known, spline functions have been used in various fields such as computer graphics, numerical analysis, image processing, trajectory planning of robot and aircraft, and data analysis in general. Recently, in (Nakata and Kano, 2003), the theory of smoothing splines is used to generate cursive characters based on an idea that the underlying writing motions become smooth. Thus splines have been studied extensively (e.g. (Wahba, 1990)), and in particular, the theory of ‘dynamic splines’ based on optimal control theory provides a unified framework for generating various types of splines (e.g. (Zhang et al., 1997)). Also, the authors studied B-splines from the viewpoint of optimal control theory (Kano et al., 2003).

One of the advantages of using spline functions is in its computational feasibilities. In particular, using B-splines as basis functions (de Boor, 1978) yields extremely simple algorithms for designing curves and surfaces. On the other hand, when we are given a set of data corrupted by noises, smoothing splines are expected to yield more feasible solutions than interpolating splines. A theoretical issue in this regard is asymptotic analyses of designed spline curves when the number of data increases. Such a problem is studied in (Egerstedt and Martin, 2003) in dynamical systems settings, namely for splines generated as an output of linear dynamical systems.

In this paper, using B-splines as basis functions, we design optimal smoothing spline curves and analyze their properties. Assuming that a number of data is given by sampling some curve \( f(t) \) with noises, we analyze statistical properties of optimal smoothing splines and derive an expression of the splines as a functional of \( f(t) \) when the number tends to infinity. Such a design and analysis method is extended to the case where \( f(t) \) is a periodic function, which can be used to model contours or shapes (Blake and Isard, 2000) of various objects.
For designing curves $x(t)$, we employ normalized, uniform B-spline function $B_k(t)$ of degree $k$ as basis functions,

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

(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 $k$ with the knot points $t_i$. In particular, by an appropriate choice of $\tau_i$‘s, arbitrary spline of degree $k$ can be designed in the interval $[t_0, t_m]$.

In the sequel, we briefly describe the normalized, uniform B-spline functions: $B_k(t)$ is defined by

$$B_k(t) = \begin{cases} N_{k-j,k}(t-j), & j \leq t \leq j + 1, \\ 0, & t \leq 0, \ k+1 \leq t. \end{cases}$$

(3)

Here the basis elements $N_{j,k}(t)$ are obtained recursively as follows (e.g. Takayama and Kano, 1995)): Let $N_{0,0}(t) \equiv 1$ and, for $i = 1,2,\cdots, k$,

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

(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 sense of $\sum_{j=0}^{k} N_{j,k}(t) = 1, \ 0 \leq t \leq 1$, and this yields $\int_{-\infty}^{\infty} B_k(t) dt = \int_{0}^{1+k} B_k(t) dt = 1$.

In particular, cubic B-spline $B_3(t)$ is frequently used in various applications, and is given by

$$B_3(t) = \begin{cases} \frac{t^3}{6}, & 0 \leq t < 1 \\ \frac{(-3t^3 + 12t^2 - 12t + 4)}{6}, & 1 \leq t < 2 \\ \frac{(3t^3 - 24t^2 + 60t - 44)}{6}, & 2 \leq t < 3 \\ \frac{(4-t)^3}{6}, & 3 \leq t < 4 \\ 0, & \text{otherwise.} \end{cases}$$

(5)

2. OPTIMAL SMOOTHING SPLINE CURVES

In this section, we present basic results on smoothing spline problems. For simplicity, we restrict ourselves to the case of $k = 3$.

Equation (1) in the case of $k = 3$ is written as

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

(6)

Suppose that we are given a set of data

$$\mathcal{D} = \{(u_i; d_i) : t_0 \leq u_1 < \cdots < u_N \leq t_m, \ d_i \in \mathbb{R}, \ i = 1, \cdots, N\},$$

(7)

and let $\tau \in \mathbb{R}^M$ be the weight vector defined by

$$\tau = \left[\tau_3 \ \tau_2 \ \cdots \ \tau_{m-1}\right]^T,$$

(8)

where $M = m+3$.

Then, a basic problem of optimal smoothing splines is to find a curve $x(t)$, or equivalently a vector $\tau \in \mathbb{R}^M$, minimizing a cost function,

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

(9)

where $\lambda(>0)$ is a smoothing parameter, $w_i(0 \leq w_i \leq 1)$ are weights for error, and the integration interval $I$ is taken as either $I = (-\infty, +\infty)$ or $I = (t_0, t_m)$.

In order to express the right hand side of (9) in terms of $\tau$, we introduce the following notations: Let a vector $b(t) \in \mathbb{R}^M$ be

$$b(t) = \left[ B_3(\alpha(t - t_{-3})) \ B_3(\alpha(t - t_{-2})) \cdots \ B_3(\alpha(t - t_{m-1})) \right]^T,$$

(10)

and a matrix $B \in \mathbb{R}^{M \times N}$ be

$$B = \left[ b(u_1) \ b(u_2) \cdots b(u_N) \right].$$

(11)

Then, we can show that the cost function is written as follows:

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

(12)

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

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

(13)

and

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

(14)

$$d = [d_1 \ d_2 \cdots d_N]^T.$$
We then see that optimal weight \( \tau \) is obtained as a solution of
\[
(\lambda Q + BWB^T)\tau = BWd. \tag{16}
\]
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 \( S = S^T \geq 0, U \) and vector \( v \) of compatible dimensions. Obviously, the solution is unique if and only if \( \lambda Q + BWB^T > 0 \). The Gramian \( Q \in \mathbb{R}^{M \times M} \) in (13) is computed explicitly. By changing integration variable, it holds that
\[
Q = \alpha^3 R. \tag{18}
\]
Here \( R \in \mathbb{R}^{M \times M} \) is defined by
\[
R = \frac{1}{6}
\begin{bmatrix}
16 & -9 & 0 & 1 \\
-9 & 16 & -9 & 0 \\
0 & -9 & 16 & -9 \\
1 & 0 & -9 & 16
\end{bmatrix}, \tag{21}
\]
and \( R_F \) for the case of \( \hat{I} = (0, m) \), is obtained by
\[
R_F = R_{\infty} - (R_- + R_+), \tag{22}
\]
where
\[
R_- = \frac{1}{6}
\begin{bmatrix}
14 & -6 & 0 & 0 \\
-6 & 8 & -3 & -3 \\
0 & 2 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}, \tag{23}
\]
and
\[
R_+ = \frac{1}{6}
\begin{bmatrix}
0 & M_{-3, M-3} & 0 & M_{-3, M-3} \\
0 & M_{-3, M-3} & 2 & -3 \\
-3 & 8 & -6 & 0 \\
0 & -6 & 14 & 0
\end{bmatrix}. \tag{24}
\]
It holds that \( Q_\infty = \alpha^3 R_\infty > 0 \) and \( Q_F = \alpha^3 R_F \geq 0 \) with rank\( R_F = M - 2 \). Thus (16) has a unique solution when \( I = (-\infty, +\infty) \). When \( I = (t_0, t_m) \), although it depends on the data points \( u_i, i = 1, \ldots, N \), there may be infinitely many solutions.

In such a case we employ the minimum Euclidean norm, which is guaranteed to be unique.

3. SMOOTHING SPLINE CURVES FOR SAMPLED DATA

We assume that the data \( d_i \) in (7) is obtained by sampling a function \( f(t) \) which is assumed to be continuous in the interval \( [t_0, t_m] \). In order to analyze asymptotic properties of spline curves as the number of data points \( N \) increases, we consider the following cost function instead of (9),
\[
J_N(\tau) = \lambda \int_{t_0}^{t_m} \left( x^{(2)}(t) \right)^2 dt + \frac{1}{N} \sum_{i=1}^{N} (x(u_i) - f(u_i))^2. \tag{25}
\]
When the data \( d_i \) is obtained by sampling the function \( f(t) \) with additive noises
\[
d_i = f(u_i) + \epsilon_i, \quad i = 1, 2, \ldots, N, \tag{26}
\]
we consider a cost function
\[
J'_N(\tau) = \lambda \int_{t_0}^{t_m} \left( x^{(2)}(t) \right)^2 dt + \frac{1}{N} \sum_{i=1}^{N} (x(u_i) - f(u_i) - \epsilon_i)^2. \tag{27}
\]
We assume that the noises are zero-mean and white, namely \( \mathbb{E}\{\epsilon_i\} = 0 \) and \( \mathbb{E}\{\epsilon_i \epsilon_j\} = \sigma^2 \delta_{ij} \) for all \( i, j \). Moreover, for analyzing the asymptotic properties, we introduce a cost function
\[
J_\epsilon(\tau) = \lambda \int_{t_0}^{t_m} \left( x^{(2)}(t) \right)^2 dt + \int_{t_0}^{t_m} (x(t) - f(t))^2 dt. \tag{28}
\]
\[
J_N(\tau) \quad \lambda Q + \frac{1}{N} BB^T \tau = \frac{1}{N} B f, \tag{29}
\]
where \( Q \) and \( B \) are given in (13) and (11), respectively, and \( f = [f(u_1) f(u_2) \cdots f(u_N)]^T \). Obviously, \( \tau_N \) minimizing \( J_N(\tau) \) is a solution of
\[
J'_N(\tau) \quad \lambda Q + \frac{1}{N} BB^T \tau = \frac{1}{N} B (f + \epsilon), \tag{30}
\]
where \( \epsilon = [\epsilon_1 \epsilon_2 \cdots \epsilon_N]^T \). On the other hand, \( J_c(\tau) \) can be written as

\[
J_c(\tau) = \tau^T(\lambda Q + R)\tau + 2\tau^T \int_{t_0}^{t_m} f(t)dt + \int_{t_0}^{t_m} f^2(t)dt,
\]

where

\[
R = \int_{t_0}^{t_m} b(t)b^T(t)dt = \alpha^{-1} R_0,
\]

\[
R_0 = \int_0^\infty b(t)b^T(t)dt.
\]

Thus optimal \( \tau_c \) denoted by \( \tau_c \) is obtained as a solution of

\[
(\lambda Q + R)\tau = \int_{t_0}^{t_m} b(t)f(t)dt.
\]

It can be shown that \( R_0 = R_0^T > 0 \), hence optimal \( \tau_c \) exists uniquely. Moreover, \( R_0 \) can be obtained explicitly as in the case of \( R_F \) in (22).

Convergence properties are established under the following assumption.

(A1) The sample points \( u_i, \; i = 1, 2, \cdots, N \), are such that

\[
\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} g(u_i) = \int_{t_0}^{t_m} g(t)dt
\]

for every continuous function \( g(t) \) in \([t_0, t_m]\).

We now have the following results for the case \( I = (-\infty, +\infty) \).

**Theorem 1.** Assume that the condition (A1) holds. Then,

(i) The optimal solutions \( \tau_N, \tau_N^c \) and \( \tau_c \) exist uniquely.

(ii) \( \tau_N \) converges to \( \tau_c \) as \( N \to \infty \).

(iii) \( E\{\tau_N^c\} = \tau_N \) and \( \tau_N^c \) converges to \( \tau_c \) as \( N \to \infty \) in mean squares sense.

(Proof) (i) As noted in the previous section, the Gramian \( Q \) in the case of \( I = (-\infty, +\infty) \), namely \( Q_\infty \), is positive-definite, and hence equations (29), (30) and (34) have unique solutions.

(ii) In (29) and (34), we show that

\[
\lim_{N \to \infty} \frac{1}{N} BB^T = R
\]

and

\[
\lim_{N \to \infty} \frac{1}{N} Bf = \int_{t_0}^{t_m} b(t)f(t)dt.
\]

Regarding the first assertion, (11) and (10) yield

\[
BB^T = \sum_{i=1}^{N} b(u_i)b^T(u_i),
\]

and denoting \( BB^T = [c_{jk}]_{j,k=3}^{m-1} \), we get

\[
c_{jk} = \sum_{i=1}^{N} B_3(\alpha(u_i - t_j))B_3(\alpha(u_i - t_k)).
\]

Then noting that the function \( g_{jk}(t) \) given by

\[
g_{jk}(t) = B_3(\alpha(t - t_j))B_3(\alpha(t - t_k))
\]

is continuous in \([t_0, t_m]\), and using the assumption (A1), it holds that

\[
\lim_{N \to \infty} \frac{1}{N} g_{jk} = \int_{t_0}^{t_m} g_{jk}(t)dt.
\]

Thus

\[
\lim_{N \to \infty} \frac{1}{N} BB^T = \lim_{N \to \infty} \left[ \frac{1}{N} c_{jk} \right]_{j,k=3}^{m-1} = \int_{t_0}^{t_m} [g_{jk}(t)]_{j,k=3}^{m-1} dt = \int_{t_0}^{t_m} b(t)b^T(t)dt = R.
\]

The second assertion (37) follows similarly by noting that \( f(t) \) is assumed to be continuous in \([t_0, t_m]\).

(iii) Taking expectations of both sides of (30) and noting \( E\{\epsilon\} = 0 \), we get

\[
\left( \lambda Q + \frac{1}{N} BB^T \right) E\{\tau\} = \frac{1}{N} Bf,
\]

and we see that \( E\{\tau_N^c\} = \tau_N \) holds. On the other hand, (30) and (38) yield

\[
\left( \lambda Q + \frac{1}{N} BB^T \right) (\tau_N^c - E\{\tau_N^c\}) = \frac{1}{N} B\epsilon.
\]

Letting

\[
P_N = E\{ (\tau_N^c - E\{\tau_N^c\}) (\tau_N^c - E\{\tau_N^c\})^T \},
\]

and using \( E\{\epsilon\epsilon^T\} = \sigma^2 I_N \), we have

\[
\left( \lambda Q + \frac{1}{N} BB^T \right) P_N \left( \lambda Q + \frac{1}{N} BB^T \right)^T = \sigma^2 \left( \frac{1}{N} BB^T \right).
\]

Noting (36), this equation in the limit of \( N \to \infty \) reduces to

\[
(\lambda Q + R)P_\infty(\lambda Q + R) = 0,
\]

where \( P_\infty(\lambda Q + R) ^T = 0. \)
and $P_\infty = 0$. Since $E(\tau_N^*) = \tau_N$, we see that $\tau_N^*$ converges to $\lim_{N \to \infty} \tau_N = \tau_c$. (Q.E.D.)

Remark 1. On the other hand, when $I = (t_0, t_m)$, the matrix $Q (= Q_F)$ has rank deficiency 2. Thus it is possible that the coefficient matrix $\lambda Q + \frac{1}{N} BB^T$ in (29) and (30) becomes singular depending on the matrix $B$, i.e. on the data points $u_i, i = 1, \ldots, N$. In such a case, there exist infinitely many solutions since these equations are guaranteed to be consistent. It is then obvious that the above theorem still holds with the understanding that we take minimum norm solutions.

4. PERIODIC SMOOTHING SPLINES

We consider to construct periodic smoothing splines. Specifically, the cost functions in previous sections are minimized subject to the continuity constraints

$$x^{(i)}(t_0) = x^{(i)}(t_m), \quad i = 0, 1, 2, \quad (39)$$

and we assume that the function $f(t)$ to be sampled satisfies $f(t_0) = f(t_m)$.

Using (6), (5) and (2), we can show that $x^{(i)}(t_0) = x^{(i)}(t_m)$ for $i = 0, 1, 2$ is written respectively as

$$\frac{1}{6} \tau - 3 + \frac{4}{6} \tau - 2 + \frac{1}{6} \tau - 1 = \frac{1}{6} \tau_{m-3} + \frac{4}{6} \tau_{m-2} + \frac{1}{6} \tau_{m-1}$$

$$- \tau - 3 + \tau - 1 = - \tau_{m-3} + \tau_{m-1}$$

$$\tau - 3 - 2 \tau - 2 + \tau - 1 = \tau_{m-3} - 2 \tau_{m-2} + \tau_{m-1},$$

yielding $\tau - 3 = \tau_{m-3}$, $\tau - 2 = \tau_{m-2}$ and $\tau - 1 = \tau_{m-1}$. Thus (39) is written as a linear constraint,

$$C^T \tau = 0, \quad (40)$$

where the matrix $C \in \mathbb{R}^{3 \times 3}$ is defined by

$$C = [ I_3 \ 0_{3,M-6} \ -I_3 ]^T. \quad (41)$$

Minimizing the cost functions subject to the constraint (40) is now a straightforward task. For the cost function $J(\tau)$ in (9), i.e. (12), we form the following Lagrangian function,

$$L(\tau, \mu) = \lambda \tau^T Q \tau + (B^T \tau - d)^T W (B^T \tau - d)$$

$$+ \mu^T (C^T \tau), \quad (42)$$

where $\mu \in \mathbb{R}^3$. Then, by taking derivatives with respect to $\tau$ and $\mu$, we get

$$2 \lambda Q \tau + 2 B W B^T \tau - 2 B W d + C \mu = 0$$

$$C^T \tau = 0, \quad (43)$$

or

$$\begin{bmatrix} \lambda Q + B W B^T C & C^T 0 \\ 0 & 1/2 \mu \end{bmatrix} = \begin{bmatrix} B W d \\ 0 \end{bmatrix}. \quad (44)$$

It can be shown that this equation is consistent, namely

$$\text{rank} \begin{bmatrix} \lambda Q + B W B^T C & \tau \\ 0 & 1/2 \mu \end{bmatrix} = \text{rank} \begin{bmatrix} \lambda Q + B W B^T C & 0 \end{bmatrix}.$$

Here, if $\lambda Q + B W B^T > 0$, then the coefficient matrix in (44) is nonsingular and the solution is unique. In case it is singular, we employ the minimum norm solution, yielding unique $\tau$.

By letting $W = \frac{1}{N} I_N$ and $d = f$ in (44), the corresponding result for the cost function $J_N(\tau)$ in (25) follows as

$$\begin{bmatrix} \lambda Q + \frac{1}{N} B W B^T & \tau \\ 0 & 1/2 \mu \end{bmatrix} = \begin{bmatrix} \frac{1}{N} B f \\ 0 \end{bmatrix}, \quad (45)$$

and the case of $J_N(\tau)$ in (27) is obtained by replacing $f$ in (45) by $f + \epsilon$. Similarly, for the cost function $J_\epsilon(\tau)$ in (28), (i.e. (31)), we obtain

$$\begin{bmatrix} \lambda Q + R C & \tau \\ C^T 0 \end{bmatrix} = \begin{bmatrix} \int_{t_0}^{t_m} b(t)f(t)dt \\ 1/2 \mu \end{bmatrix}. \quad (46)$$

Here, noting $R > 0$, we can show that this coefficient matrix is nonsingular, and the solution exists uniquely.

Finally we examine the properties of solutions for cost functions $J_N(\tau)$ and $J_N(\tau)$. By noting the relations (36) and (37), we readily see that the same assertions as in Theorem 1 and Remark 1 hold also for the present periodic case.

5. SIMULATION STUDIES

We examine performances of smoothing splines for a periodic case.

Let $(p(t), q(t))$ be a periodic curve with period 36 in $pq$-plane,

$$(p(t), q(t)) = \left(3 + r(t) \cos \frac{2\pi t}{36}, \ 3 + r(t) \sin \frac{2\pi t}{36}\right), \quad (47)$$

with $r(t) = 2 + \sin \frac{10\pi t}{36}$, and let a periodic function $f(t)$ to be sampled be given by

$$f(t) = \sqrt{p^2(t) + q^2(t)}, \quad 0 \leq t \leq 36. \quad (48)$$

Moreover, in (6), we set $m = 36, \ a = 1, \ t_0 = 0$ and $t_m = 36$. Thus the knot points $t_i$ are taken as integers as $t_i = i$. 
We applied the method described in the previous section to the data obtained by sampling the curve \( f(t) \). Here the number of data points \( N \) is set as \( N = 30 \), and they are equally spaced in the interval \([0, 36]\). The noise magnitude is set as \( \sigma = 0.02 \) and the integration interval as \( I = [t_0, t_m] = [0, 36] \).

The smoothing parameter \( \lambda \) is estimated by employing the so-called 'leaving-out-one' method (Wahba, 1990): An optimum \( \lambda \) as the minimizer of ordinary cross-validation function was obtained as \( \lambda = 0.0178 \).

The optimal weights \( \tau_N^c \) and \( \tau_c \) are computed, and Fig.1 shows the corresponding curves \( x_N^c(t) \) (black line) and \( x_c(t) \) (green line) together with the data points (asterisks) and the original curve \( f(t) \) (dashed red line). Note that \( x_c(t) \) and \( f(t) \) are almost indistinguishable, implying that \( x_N^c(t) \) can approximates \( f(t) \) almost perfectly as the number of data points \( N \) is increased.

The corresponding results are plotted in the \( pq \)-plane. On recovering \((p, q)\) information from the curve \( x_N^c(t) \) (and \( x_c(t) \)), we assume that they are related as in (47) and (48). Specifically, the equations used for \( x_N^c(t) \), for example, are

\[
(p_N^c(t), q_N^c(t)) = (x_N^c(t) \sin \theta(t), x_N^c(t) \cos \theta(t)),
\]

where \( \theta(t) \) is computed using the two-argument arctangent function \( \text{atan2}(\cdot, \cdot) \) as

\[
\theta(t) = \text{atan2} \left( 3 + r(t) \cos \frac{2 \pi t}{36}, 3 + r(t) \sin \frac{2 \pi t}{36} \right).
\]

6. CONCLUDING REMARKS

We considered a problem of designing optimal smoothing spline curves using B-splines as basis functions. For given data \((t_i, f(t_i) + \epsilon_i), i = 1, \cdots, N\), the expression for optimal smoothing curve is derived in the limit of \( N \to \infty \). It is then shown that, under a very natural assumption, optimal smoothing splines converge to this curve as \( N \to \infty \). The design and analysis methods are extended to the case of periodic splines. The results for the case of periodic splines are verified numerically for contour synthesizing problem. As the applications, we are planning to model contours or shapes of various objects including living bodies.

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