2011 50th IEEE Conference on Decision and Control and
European Control Conference (CDC-ECC)
Orlando, FL, USA, December 12-15, 2011

Optimal Smoothing Spline Surfaces with Constraints on Derivatives

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Abstract— **In this paper, we consider the problem of constructing optimal smoothing spline surfaces with constraints on their derivatives. The spline surfaces are constituted by using normalized uniform B-splines as the basis functions. We then show that the derivatives of spline surface can be expressed by using B-splines of lower degree, and that the corresponding control points are computed as two-dimensional differences of original control point array. This enables us to treat systematically equality and/or inequality constraints over arbitrary knot point regions on partial derivatives of arbitrary degree. Then, the problem of optimal smoothing spline surfaces with constraints is reduced to convex quadratic programming problem. The performance is examined numerically by approximating monotone and concave surfaces.**

I. INTRODUCTION

Even though the traditional approximating or interpolating spline curves and surfaces are well behaved for wide range of applications (see e.g. [1]), we frequently face the problems where we need to impose various types of constraints on the splines (see e.g. [2], [3]). In particular, the constraints for preserving the properties on derivatives, e.g. monotonicity and convexity, etc., are very important in practical applications of various fields – such as robotics, biochemistry, pharmacology, statistics and finance, etc [4].

It is relatively easy to construct spline curves and surfaces with constraints on the derivatives at isolated points (see e.g. [2], [5], [6]). The problem of constructing spline curves and surfaces with such constraints has been reduced to a quadratic programming problem and solved. On the other hand, the problem of imposing the constraints on some interval or region seems to lead to an infinite dimensional problem and not be easily solved in general. Thus, most of the related works have been done for the case of splines with specific degree. For example, Egerstedt and Martin in [7] have developed the method of constructing monotone splines by the control theoretic approach. Then, they formulated and solved the problem as a dynamic programming problem but the method is specific to the cubic splines. Meyer in [8] has not only constructed monotone splines but also extended the construction to the case of convex constraints. Her construction is also limited to the cubic splines. While these are for spline curves, similar problems for the spline surface have been studied by various authors (see e.g. [9], [10], [11], [12], [13]), but they are also specific to the cubic case or lower.

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Motivated by these works, the authors have recently developed a method for constructing optimal smoothing spline curves with constraints on their derivatives [14]. In particular, we have shown that B-spline approach enables us to yield systematic treatments and solutions for problems with equality and inequality constraints over intervals on derivatives of arbitrary degree. Moreover, a part of such results using B-spline approach have been extended to the case of surfaces [6], but the constraints on their derivatives have not been treated there.

In this paper, we concentrate on the constraints on the derivatives of spline surfaces. Specifically, based on our studies in [6] and [14], we develop a systematic method of constructing optimal smoothing spline surfaces with equality and/or inequality constraints on their partial derivatives of arbitrary degree over arbitrary knot point regions. The splines are constructed by employing normalized uniform B-splines as the basis functions. First, we develop a formula for expressing the derivatives of spline surfaces together with a concise expression of the underlying control points. We then show that the constraints on derivatives can be systematically added and the construction of spline surfaces becomes convex quadratic programming problem. The performance is examined numerically by approximating monotone and concave surfaces.

Here are the principal symbols used in this paper: ∇^2 and $\otimes$ denote the Laplacian operator and the Kronecker product, respectively. In addition, 'vec' denotes the vec-function, i.e. for a matrix $A = [a_1\ a_2 \cdots\ a_n] \in \mathbf{R}^{m\times n}$ with $a_i \in \mathbf{R}^m$, vec $A = [a_1^T\ a_2^T\ \cdots\ a_n^T]^T \in \mathbf{R}^{mn}$ (see e.g. [15]).

II. OPTIMAL SPLINE SURFACES

As preliminaries, we present B-spline surfaces and the optimal design method of smoothing surfaces.

A. B-Spline Surfaces

Using normalized, uniform B-spline function as the basis function, we construct surfaces $x(s,t)$ on a domain $\mathscr{D} = [s_0, s_{m_1}] \times [t_0, t_{m_2}] \subset \mathbf{R}^2$. Then, $x(s,t)$ is given by

$$x(s,t) = \sum_{i=-k}^{m_1-1}\sum_{j=-k}^{m_2-1} \tau_{i,j} B_k(\alpha(s-s_i))B_k(\beta(t-t_j)), \quad (1)$$

where $\tau_{i,j}$ are the weighting coefficients called control points, $\alpha,\ \beta(>0)$ are constants, $m_1,\ m_2(>2)$ are integers, and s_i's, t_j's are equally spaced knot points with

$$s_{i+1} - s_i = \frac{1}{\alpha}, \quad t_{j+1} - t_j = \frac{1}{\beta}. \quad (2)$$

Here, $B_k(t)$ denotes normalized uniform B-spline of degree k 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 $N_{j,k}(t)$ $(j=0,1,\cdots,k)$, $0 \le t \le 1$ can be obtained by a recursive algorithm (see e.g. [16]). Then, it is known that $B_k(t)$ is a piece-wise polynomial of degree k with integer knot points and is $k-1$ times continuously differentiable.

For the sake of later reference, we introduce $(k+1)$-dimensional vectors $N_k(t)$ and $h_k(t)$ as

$$N_k(t) = \begin{bmatrix} N_{0,k}(t) & N_{1,k}(t) & \cdots & N_{k,k}(t) \end{bmatrix}^T \tag{4}$$

$$h_k(t) = \begin{bmatrix} t^k & t^{k-1} & \cdots & 1 \end{bmatrix}^T. \tag{5}$$

In addition, let $S_k \in \mathbf{R}^{(k+1)\times(k+1)}$ be a matrix whose i-th row consists of the coefficients of the polynomial $N_{i-1,k}(t)$. Then, $N_k(t)$ is written as

$$N_k(t) = S_k h_k(t). \tag{6}$$

It can be shown that the matrix S_k can be obtained recursively as follows: Letting $S_0 = 1$, compute $S_i \in \mathbf{R}^{(i+1)\times(i+1)}$ for $i = 1,2,\cdots,k$ by

$$S_i = \frac{1}{i}\left(\begin{bmatrix} 0_{i+1} & \Gamma_i S_{i-1} \end{bmatrix} + \begin{bmatrix} \Delta_i S_{i-1} & 0_{i+1} \end{bmatrix}\right), \tag{7}$$

where the matrices $\Gamma_i, \Delta_i \in \mathbf{R}^{(i+1)\times i}$ are defined as

$$\Gamma_i = \begin{bmatrix} 1 & & & & \\ i-1 & 2 & & & \\ & i-2 & 3 & & \\ & & \ddots & \ddots & \\ & & & 1 & i \\ & & & 0 & 0 \end{bmatrix}, \tag{8}$$

$$\Delta_i = \begin{bmatrix} -1 & & & & \\ 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & \ddots & \\ & & & 1 & -1 \\ & & & & 1 \end{bmatrix}. \tag{9}$$

Here the empty spaces denote zero entries.

B. Optimal Smoothing Surfaces

Using B-spline surfaces in (1), the problem of constructing optimal smoothing surfaces reduces to one of determining control points $\tau_{i,j}$ [16]. Here we confine our attention to express the cost functions for the optimal design.

Suppose that we are given a set of data

$$\left\{(u_i, v_j; d_{ij}) : u_i \in [s_0, s_{m_1}], v_i \in [t_0, t_{m_2}], d_{ij} \in \mathbf{R}, \right. \\ \left. i = 1,2,\cdots,N_1,\ j=1,2,\cdots,N_2\right\} \tag{10}$$

and let $\tau \in \mathbf{R}^{M_1 \times M_2}$ be the control point matrix defined by

$$\tau = \begin{bmatrix} \tau_{-k,-k} & \tau_{-k,-k+1} & \cdots & \tau_{-k,m_2-1} \\ \tau_{-k+1,-k} & \tau_{-k+1,-k+1} & \cdots & \tau_{-k+1,m_2-1} \\ \vdots & \vdots & \cdots & \vdots \\ \tau_{m_1-1,-k} & \tau_{m_1-1,-k+1} & \cdots & \tau_{m_1-1,m_2-1} \end{bmatrix} \tag{11}$$

with $M_1 = m_1 + k$ and $M_2 = m_2 + k$. Then a standard problem is to find such a τ minimizing the cost function

$$J(\tau) = \lambda \int_{I_1}\int_{I_2} \left(\nabla^2 x(s,t)\right)^2 ds dt + \sum_{i=1}^{N_1}\sum_{j=1}^{N_2} w_{ij}(x(u_i,v_j) - d_{ij})^2 \tag{12}$$

with $I_1 = [s_0, s_{m_1}]$, $I_2 = [t_0, t_{m_2}]$. Here, $\lambda (>0)$ is a smoothing parameter, and w_{ij} $(0 \le w_{ij} \le 1)$ are the weights for approximation errors.

By employing Kronecker product and vec-function, $x(s,t)$ in (1) is rewritten as

$$x(s,t) = (b_2(t) \otimes b_1(s))^T \hat{\tau} \tag{13}$$

with $\hat{\tau} \in \mathbf{R}^{M_1 M_2}$, $b_1(s) \in \mathbf{R}^{M_1}$ and $b_2(t) \in \mathbf{R}^{M_2}$ defined by

$$\hat{\tau} = \text{vec}\ \tau \tag{14}$$

$$b_1(s) = [B_k(\alpha(s - s_{-k}))\ B_k(\alpha(s - s_{-k+1}))\ \cdots \\ \cdots\ B_k(\alpha(s - s_{m_1-1})]^T, \tag{15}$$

$$b_2(t) = [B_k(\beta(t - t_{-k}))\ B_k(\beta(t - t_{-k+1}))\ \cdots \\ \cdots\ B_k(\beta(t - t_{m_2-1}))]^T. \tag{16}$$

Then, utilizing the expression in (13), the cost function $J(\tau)$ in (12) can be rewritten as a quadratic function in terms of $\hat{\tau}$ (see e.g. [16] for details),

$$J(\hat{\tau}) = \hat{\tau}^T(\lambda Q + \Gamma W \Gamma^T)\hat{\tau} - 2\hat{\tau}^T \Gamma W d + d^T W d, \tag{17}$$

where $Q \in \mathbf{R}^{M_1 M_2 \times M_1 M_2}$ is a Gram matrix defined by

$$Q = \int_{I_1}\int_{I_2} \left(\nabla^2 (b_2(t) \otimes b_1(s))\right)\left(\nabla^2 (b_2(t) \otimes b_1(s))\right)^T ds dt. \tag{18}$$

Moreover, in (17), the matrix $\Gamma \in \mathbf{R}^{M_1 M_2 \times N_1 N_2}$ is defined

$$\Gamma = \bar{B}_2 \otimes \bar{B}_1 \tag{19}$$

with matrices $\bar{B}_1 \in \mathbf{R}^{M_1 \times N_1}$ and $\bar{B}_2 \in \mathbf{R}^{M_2 \times N_2}$ defined by

$$\bar{B}_1 = \begin{bmatrix} b_1(u_1) & b_1(u_2) & \cdots & b_1(u_{N_1}) \end{bmatrix}, \\ \bar{B}_2 = \begin{bmatrix} b_2(v_1) & b_2(v_2) & \cdots & b_2(v_{N_2}) \end{bmatrix}. \tag{20}$$

Also, $W \in \mathbf{R}^{N_1 N_2 \times N_1 N_2}$ and $d \in \mathbf{R}^{N_1 N_2}$ are given by

$$W = \text{diag}\{w_{11},\ w_{21},\ \cdots,\ w_{N_1 1},\ \cdots, \\ w_{1N_2},\ w_{2N_2},\ \cdots,\ w_{N_1 N_2}\}$$

$$d = [\ d_{11},\ d_{21},\ \cdots,\ d_{N_1 1},\ \cdots, \\ d_{1N_2},\ d_{2N_2},\ \cdots,\ d_{N_1 N_2}]^T. \tag{21}$$

Notice here that $\lambda Q + \Gamma W \Gamma^T$ in (17) is positive-semidefinite, i.e. $\lambda Q + \Gamma W \Gamma^T \ge 0$, since $\lambda > 0$, $Q \ge 0$ and $W \ge 0$, and hence the cost $J(\hat{\tau})$ in (17) is a convex function.

III. Optimal Spline Surfaces with Constraints on Derivatives

For the optimal smoothing spline surfaces $x(s,t)$ of degree k as described in the previous section, we consider to impose the following condition on its partial derivatives

$$\frac{\partial^{l_1+l_2}}{\partial s^{l_1}\partial t^{l_2}}x(s,t) \geq c \quad \forall (s,t) \in \mathscr{D}_{\kappa,\mu}, \tag{22}$$

where $0 \leq l_1, l_2 \leq k$ and c is a given constant. Also, $\mathscr{D}_{\kappa,\mu}$ is some knot point region $\mathscr{D}_{\kappa,\mu} = [s_\kappa, s_{\kappa+1}] \times [t_\mu, t_{\mu+1}]$ for $\kappa = 0,1,\cdots,m_1-1$ and $\mu = 0,1,\cdots,m_2-1$. Setting $(l_1,l_2) = (0,1),(1,0)$ and $c=0$ yields monotone spline surfaces, while $(l_1,l_2) = (0,2),(2,0),(1,1)$ and $c=0$ yields concave spline surfaces.

Note that such constraints for each knot point region $\mathscr{D}_{\kappa,\mu}$ allow us more flexible treatment of constraints over regions, such as the surface being convex on some region and concave on another. Also, the above inequality '$\geq$' can be readily replaced with '$\leq$' or equality '$=$', as we will see in the subsequent development.

Our task here is to derive the expression of such constraints in terms of the control points $\tau_{i,j}$. In the sequel, we first develop basic formula for expressing the partial derivatives of splines (Section III-A). We then express constraints on the derivatives in terms of control points $\tau_{i,j}$ and reduce the problem to quadratic programming problem (Section III-B).

A. Formula for Derivatives on Spline Surfaces

We first develop basic formula in order to derive the expression of constraints on the derivatives. Now, we notice that $x(s,t)$ is constituted by a product of two piecewise polynomials. We thus examine the polynomial in each knot point region $\mathscr{D}_{\kappa,\mu} = [s_\kappa, s_{\kappa+1}] \times [t_\mu, t_{\mu+1}]$ for $\kappa = 0,1,\cdots,m_1-1$ and $\mu = 0,1,\cdots,m_2-1$.

For the region $\mathscr{D}_{\kappa,\mu}$, the spline surface $x(s,t)$ in (1) is written as

$$x(s,t) = \sum_{i=-k+\kappa}^{\kappa} \sum_{j=-k+\mu}^{\mu} \tau_{i,j} B_k(\alpha(s-s_i)) B_k(\beta(t-t_j)), \tag{23}$$

and, by (3), we get

$$x(s,t) = \sum_{i=0}^{k}\sum_{j=0}^{k} \tau_{\kappa-k+i,\mu-k+j} N_{i,k}(\alpha(s-s_\kappa)) N_{j,k}(\beta(t-t_\mu)). \tag{24}$$

In addition, we introduce new variables u and v defined as

$$u = \alpha(s-s_\kappa), \; v = \beta(t-t_\mu). \tag{25}$$

Then, the region $\mathscr{D}_{\kappa,\mu}$ is normalized to the unit region $\mathscr{E} = [0,1]\times[0,1]$ for (u,v). Now $x(s,t)$ is expressed in terms of (u,v) as $x(s,t) = \hat{x}(u,v)$ with

$$\hat{x}(u,v) = \sum_{i=0}^{k}\sum_{j=0}^{k} \tau_{\kappa-k+i,\mu-k+j} N_{i,k}(u) N_{j,k}(v). \tag{26}$$

Moreover, let $x^{(l_1,l_2)}(s,t)$ be the derivatives of $x(s,t)$ as

$$x^{(l_1,l_2)}(s,t) = \frac{\partial^{l_1+l_2}}{\partial s^{l_1}\partial t^{l_2}} x(s,t), \tag{27}$$

and $\hat{x}^{(l_1,l_2)}(u,v)$ be defined similarly. Then, $x(s,t)$ and $\hat{x}(u,v)$ are related by

$$x^{(l_1,l_2)}(s,t) = \alpha^{l_1}\beta^{l_2}\hat{x}^{(l_1,l_2)}(u,v), \; l_1,l_2 = 0,1,\cdots. \tag{28}$$

Now letting $T_{[\kappa-k,\kappa]\times[\mu-k,\mu]} \in \mathbf{R}^{(k+1)\times(k+1)}$ be the submatrix of τ in (11) as

$$T_{[\kappa-k,\kappa]\times[\mu-k,\mu]} = \begin{bmatrix} \tau_{\kappa-k,\mu-k} & \tau_{\kappa-k,\mu-(k-1)} & \cdots & \tau_{\kappa-k,\mu} \\ \tau_{\kappa-(k-1),\mu-k} & \tau_{\kappa-(k-1),\mu-(k-1)} & \cdots & \tau_{\kappa-(k-1),\mu} \\ \vdots & \vdots & & \vdots \\ \tau_{\kappa,\mu-k} & \tau_{\kappa,\mu-(k-1)} & \cdots & \tau_{\kappa,\mu} \end{bmatrix}, \tag{29}$$

then $\hat{x}^{(l_1,l_2)}(u,v)$ in (28) is expressed as

$$\begin{aligned} \hat{x}^{(l_1,l_2)}(u,v) &= \sum_{i=0}^{k}\sum_{j=0}^{k} \tau_{\kappa-k+i,\mu-k+j} N_{i,k}^{(l_1)}(u) N_{j,k}^{(l_2)}(v) \\ &= N_k^{(l_1)}(u)^T T_{[\kappa-k,\kappa]\times[\mu-k,\mu]} N_k^{(l_2)}(v). \end{aligned} \tag{30}$$

Here, it was shown in [14] that the derivatives of basis elements $N_k(t)$ of splines in (4) are related to lower order elements by the matrix Δ_i in (9) as follows:

Lemma 1: The l-th derivatives of vector $N_i(t)$ is given by

$$N_i^{(l)}(t) = \Delta_{[i,i-l+1]} N_{i-l}(t) \tag{31}$$

where $\Delta_{[i_1,i_2]} \in \mathbf{R}^{(i_1+1)\times i_2}$ is defined for $i_1 \geq i_2$ by

$$\Delta_{[i_1,i_2]} = \prod_{\nu=i_1}^{i_2} \Delta_\nu = \Delta_{i_1}\Delta_{i_1-1}\cdots\Delta_{i_2}. \tag{32}$$

By this lemma, it is shown that the derivatives of surface, i.e. $\hat{x}^{(l_1,l_2)}(u,v)$ in (30), is represented by the basis elements $N_{i,k'_p}(u)$, $(i=0,1,\cdots,k'_p,\; p=1,2)$ of degree k'_p, where $k'_p = k - l_p$. We thus have

$$\begin{aligned} \hat{x}^{(l_1,l_2)}(u,v) &= \sum_{i=0}^{k'_1}\sum_{j=0}^{k'_2} \phi_{\kappa-k'_1+i,\mu-k'_2+j} N_{i,k'_1}(u) N_{j,k'_2}(v) \\ &= N_{k'_1}(u)^T \Phi_{[\kappa-k'_1,\kappa]\times[\mu-k'_2,\mu]} N_{k'_1}(u), \end{aligned} \tag{33}$$

where $\Phi_{[\kappa-k'_1,\kappa]\times[\mu-k'_2,\mu]} \in \mathbf{R}^{(k'_1+1)\times(k'_2+1)}$ is defined by

$$\Phi_{[\kappa-k'_1,\kappa]\times[\mu-k'_2,\mu]} = \begin{bmatrix} \phi_{\kappa-k'_1,\mu-k'_2} & \phi_{\kappa-k'_1,\mu-(k'_2-1)} & \cdots & \phi_{\kappa-k'_1,\mu} \\ \phi_{\kappa-(k'_1-1),\mu-k'_2} & \phi_{\kappa-(k'_1-1),\mu-(k'_2-1)} & \cdots & \phi_{\kappa-(k'_1-1),\mu} \\ \vdots & \vdots & & \vdots \\ \phi_{\kappa,\mu-k'_2} & \phi_{\kappa,\mu-(k'_2-1)} & \cdots & \phi_{\kappa,\mu} \end{bmatrix}. \tag{34}$$

From (30), (31) and (33), we see that the matrix Φ in (34) is related to T in (29) by

$$\Phi_{[\kappa-k'_1,\kappa]\times[\mu-k'_2,\mu]} = \Delta_{[k,k-l_1+1]}^T T_{[\kappa-k,\kappa]\times[\mu-k,\mu]} \Delta_{[k,k-l_2+1]}. \tag{35}$$

In terms of vec-functions,

$$\begin{aligned} \hat{T}_{[\kappa-k,\kappa]\times[\mu-k,\mu]} &= \text{vec } T_{[\kappa-k,\kappa]\times[\mu-k,\mu]} \\ \hat{\Phi}_{[\kappa-k'_1,\kappa]\times[\mu-k'_2,\mu]} &= \text{vec } \Phi_{[\kappa-k'_1,\kappa]\times[\mu-k'_2,\mu]}, \end{aligned}$$

this relation is written as

$$\begin{aligned}&\hat{\Phi}_{[\kappa-k_1',\kappa]\times[\mu-k_2',\mu]}\\ &= \left(\Delta_{[k,k-l_2+1]}\otimes\Delta_{[k,k-l_1+1]}\right)^T\hat{T}_{[\kappa-k,\kappa]\times[\mu-k,\mu]} \quad (36)\end{aligned}$$

since vec $(AXB)=(B^T\otimes A)$vec X and $(A\otimes B)^T=A^T\otimes B^T$ in general.

Based on (35), we can show that the coefficients $\phi_{i,j}$ in (33) (i.e. the elements of Φ matrix) are determined in terms of $\tau_{i,j}$ in (30) (i.e. the elements of T matrix) as follows, where we introduced shift operators z_1 and z_2 such that

$$z_1^{i'}z_2^{j'}\tau_{i,j}=\tau_{i+i',j+j'}. \quad (37)$$

Lemma 2: The derivative $x^{(l_1,l_2)}(s,t)$ of spline surface $x(s,t)$ in (23) is expressed as spline surface in (28) and (33), where the control points $\phi_{i,j}$ $(\kappa-k_1'\le i\le\kappa,\mu-k_2'\le j\le\mu)$ in (33) are given in terms of $\tau_{i,j}$ by

$$\phi_{i,j}=(1-z_1^{-1})^{l_1}(1-z_2^{-1})^{l_2}\tau_{i,j}. \quad (38)$$

This lemma shows that $\phi_{i,j}$ is obtained from $\tau_{i,j}$ as the l_1-th and l_2-th backward difference in i and j respectively. When $l_1=l_2=1$, for example, we have $\phi_{i,j}=(1-z_1^{-1})(1-z_2^{-1})\tau_{i,j}=(1-z_1^{-1})(\tau_{i,j}-\tau_{i,j-1})=(\tau_{i,j}-\tau_{i,j-1})-(\tau_{i-1,j}-\tau_{i-1,j-1})$.

Using (25), (28) and (33), we get

$$x^{(l_1,l_2)}(s,t)=\alpha^{l_1}\beta^{l_2}\sum_{i=0}^{k_1'}\sum_{j=0}^{k_2'}\phi_{\kappa-k_1'+i,\mu-k_2'+j}N_{i,k_1'}(u)N_{j,k_2'}(v) \quad (39)$$

for knot point region $\mathscr{D}_{\kappa,\mu}=[s_\kappa,s_{\kappa+1}]\times[t_\mu,t_{\mu+1}]$ with $\kappa=0,1,\cdots,m_1-1$ and $\mu=0,1,\cdots,m_2-1$. The derivative of $x(s,t)$ in (1) is then expressed in terms of B-splines as

$$\begin{aligned}&x^{(l_1,l_2)}(s,t)\\ &= \alpha^{l_1}\beta^{l_2}\sum_{i=-k_1'}^{m_1-1}\sum_{j=-k_2'}^{m_2-1}\phi_{i,j}B_{k_1'}(\alpha(s-s_i))B_{k_2'}(\beta(t-t_j)).\end{aligned} \quad (40)$$

By Lemma 2, we thus have a nice property that the partial derivative $x^{(l_1,l_2)}(s,t)$ of spline surface is determined as spline surface with control points $\phi_{i,j}$ obtained as l_1-th and l_2-th differences of original control points $\tau_{i,j}$ for $x(s,t)$ in i and j respectively.

B. Constraints on Derivatives

We are now in the position to state the constraint in (22) in terms of the control points $\tau_{i,j}$. From the formulations in Section III-A, we have the following proposition.

Proposition 1: If the control points $\phi_{i,j}$ given by (38) satisfy

$$\phi_{i,j}\ge\frac{c}{\alpha^{l_1}\beta^{l_2}} \quad (41)$$

for $i=\kappa-k_1',\kappa-k_1'+1,\cdots,\kappa,\ j=\mu-k_2',\mu-k_2'+1,\cdots,\mu$, then the spline surface $x(s,t)$ satisfies the constraint (22).

This readily follows from (39) and the fact that $\sum_{j=0}^{k}N_{j,k}(t)=1,\ N_{j,k}(t)\ge 0,\ 0\le t\le 1,\ j=0,1,\cdots,k$ for any k.

Introducing a vector $\mathbf{1}_i=[1\ 1\ \cdots\ 1]^T\in\mathbf{R}^i$, the constraint (41) is written as

$$\hat{\Phi}_{[\kappa-k_1',\kappa]\times[\mu-k_2',\mu]}\ge\frac{c}{\alpha^{l_1}\beta^{l_2}}\mathbf{1}_{(k_1'+1)(k_2'+1)}, \quad (42)$$

and (36) gives the expression in terms of original control points $\tau_{i,j}$ as

$$\begin{aligned}&\left(\Delta_{[k,k-l_2+1]}\otimes\Delta_{[k,k-l_1+1]}\right)^T\hat{T}_{[\kappa-k,\kappa]\times[\mu-k,\mu]}\\ &\ge \frac{c}{\alpha^{l_1}\beta^{l_2}}\mathbf{1}_{(k_1'+1)(k_2'+1)}.\end{aligned} \quad (43)$$

It can be shown that the constraint (43) is readily extended to arbitrarily knot point region, say $[s_\kappa,s_{\kappa+n_1}]\times[t_\mu,t_{\mu+n_2}]$ for $n_1,n_2\ge 1$, as

$$\begin{aligned}&\left(\Delta_{[k+n_2+1,k-l_2+1]}\otimes\Delta_{[k+n_2-1,k-l_1+1]}\right)^T\\ &\times\ \hat{T}_{[\kappa-k,\kappa+n_1-1]\times[\mu-k,\mu+n_2-1]}\ge\frac{c}{\alpha^{l_1}\beta_{l_2}}\mathbf{1}_{(k_1'+n_1)(k_2'+n_2)}.\end{aligned} \quad (44)$$

In particular, when we want to impose the constraint (22) over the entire domain $\mathscr{D}$, namely $x^{(l_1,l_2)}(s,t)\ge c,\ \forall(s,t)\in[s_0,s_{m_1}]\times[t_0,t_{m_2}]$, then letting $\kappa,\mu=0$ and $n_i=m_i$ for $i=1,2$ in (44) yields the constraint on the control point vector $\hat{\tau}(=\text{vec }\tau)$ in (14) as

$$\begin{aligned}&\left(\Delta_{[k+m_2-1,k+m_2-l_2]}\otimes\Delta_{[k+m_1-1,k+m_1-l_1]}\right)^T\hat{\tau}\\ &\ge \frac{c}{\alpha^{l_1}\beta^{l_2}}\mathbf{1}_{(k_1'+m_1)(k_2'+m_2)}\end{aligned} \quad (45)$$

since $\hat{T}_{[-k,m_1-1]\times[-k,m_2-1]}=\hat{\tau}$ by (11).

We now have a method of describing equality and inequality constraints on all the derivatives of spline surfaces over arbitrary knot point region. In addition, constraints at isolated points and integral values of spline surfaces were developed previously in [6] as linear constraints on the control points.

Thus, using the expression of cost $J(\hat{\tau})$ in (17), the optimal constrained spline problems can be formulated as convex quadratic programming problems of the following form:

$$\min_{\hat{\tau}\in\mathbf{R}^{M_1M_2}}J(\hat{\tau})=\frac{1}{2}\hat{\tau}^TG\hat{\tau}+g^T\hat{\tau} \quad (46)$$

subject to the constraints specified in general as

$$A\hat{\tau}=p,\ f_1\le E\hat{\tau}\le f_2,\ h_1\le\hat{\tau}\le h_2, \quad (47)$$

for some matrices and vectors of appropriate dimensions. A very efficient numerical algorithm is available for this purpose (see e.g. [17]).

IV. Numerical Examples

We examine the performance of design method in the previous sections numerically. As examples, we here consider the two problems of approximating nonnegative monotone surface (Section IV-A) and concave surface (Section IV-B). In all the cases, cubic splines, i.e. $k=3$, are used.

A. Approximation of Monotone Surface

We approximate a monotone test function $f(s,t)$ in $\mathscr{D} = [s_0, s_{m_1}] \times [t_0, t_{m_2}] = [0,10] \times [0,10]$, where $f(s,t)$ is the so-called sigmoidal function used in [9],

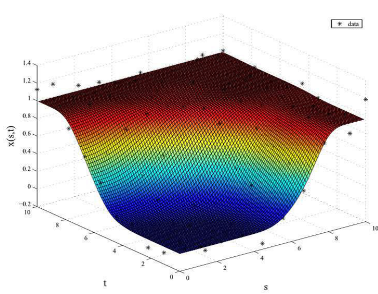
$$f(s,t) = \left(1 + 2e^{-3(r-6.7)}\right)^{-\frac{1}{2}} \tag{48}$$

with $r = \sqrt{s^2+t^2}$. The data (u_i, v_j, d_{ij}), $i = 1,2,\cdots,N_1$, $j = 1,2,\cdots,N_2$ in (10) is generated by sampling $f(s,t)$ at 100 ($= N_1 N_2 = 10 \times 10$) points with additive Gaussian white noise of zero mean and standard deviation 0.1. Also, u_i, v_j are equally spaced in $\mathscr{D}$, and $d_{ij} = f(u_i, v_j)$. The design parameters are set as $\alpha = \beta = 1$ and $m_1 = m_2 = 10$ in (1), an optimal smoothing spline surface $x(s,t)$ is computed based on the criterion (12) with $\lambda = 10^{-3}$ and $w_{ij} = 1/N_1 N_2\ \forall i, j$. On designing the surface $x(s,t)$, we imposed the inequality constraints

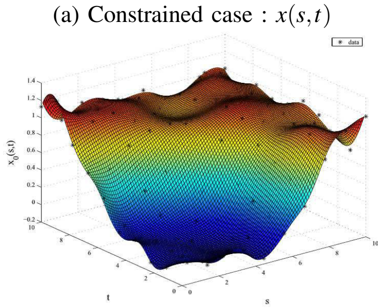
$$0 \le x(s,t) \le 1,\ x^{(1,0)}(s,t) \ge 0,\ x^{(0,1)}(s,t) \ge 0 \quad \forall (s,t) \in \mathscr{D}. \tag{49}$$

For specifying the constraints in terms of the control point vector $\hat{\tau}$, we employ the method in [6] for $0 \le x(s,t) \le 1$ and in Section III for other constraints.

The results are shown in Figure 1, where the data points (u_i, v_j, d_{ij}) are shown by asterisks (*), and the designed spline surface $x(s,t)$ is plotted in Figure 1 (a). Also, Figure 1 (b) shows an optimal smoothing spline $x_0(s,t)$ obtained without the constraints (49). The corresponding derivatives $x^{(1,0)}(s,t)$ and $x_0^{(1,0)}(s,t)$ are shown in Figure 2. We conclude that the constrained surface $x(s,t)$ results in satisfactory approximation of original one $f(s,t)$ while preserving the monotone nondecreasing property specified as (49), which is not the case with the surface $x_0(s,t)$.

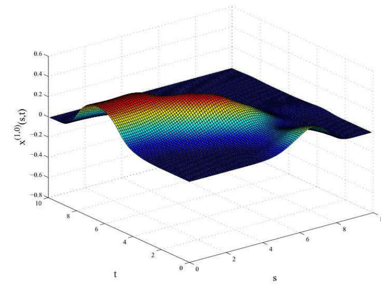


(a) Constrained case : $x(s,t)$

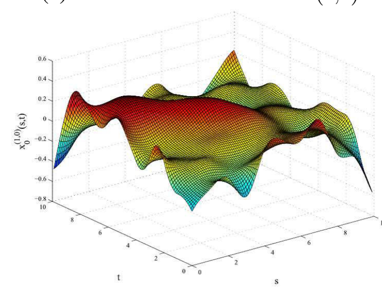


(b) Unconstrained case : $x_0(s,t)$

Fig. 1. Data points (*), (a) constrained and (b) unconstrained smoothing spline surfaces $x(s,t)$ and $x_0(s,t)$.



(a) Constrained case : $x^{(1,0)}(s,t)$



(b) Unconstrained case : $x_0^{(1,0)}(s,t)$

Fig. 2. Corresponding derivatives (a) $x^{(1,0)}(s,t)$ and (b) $x_0^{(1,0)}(s,t)$ of smoothing spline surfaces.

B. Approximation of Concave Surface

Next, we approximate the following concave function

$$\begin{aligned} f(s,t) &= \frac{1}{8-\sqrt{23.5}} \\ &\quad \times \sqrt{64 - 81\left((0.1s-0.5)^2 + (0.1t-0.5)^2\right)} \end{aligned} \tag{50}$$

in $\mathscr{D} = [s_0, s_{m_1}] \times [t_0, t_{m_2}] = [0,10] \times [0,10]$. This is a part of spherical surface used in [10], and the constraints are

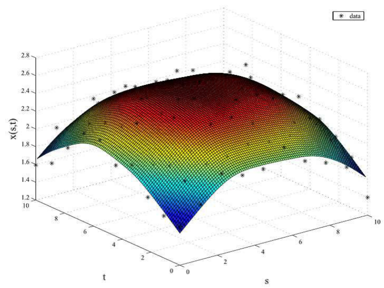
$$x^{(0,2)}(s,t) \le 0,\ x^{(1,1)}(s,t) \le 0,\ x^{(2,0)}(s,t) \le 0 \quad \forall (s,t) \in \mathscr{D}. \tag{51}$$

By employing the method in Section III, the constraints (51) are specified in terms of the control point vector $\hat{\tau}$. The data (u_i, v_j, d_{ij}) are generated by sampling $f(s,t)$ at 100 ($= N_1 N_2 = 10 \times 10$) equally spaced points (u_i, v_j) in $\mathscr{D}$ with additive Gaussian white noise of zero mean and standard deviation 0.1. The design parameters for smoothing are set as $\alpha = \beta = 1$, $m_1 = m_2 = 10$, $\lambda = 10^{-3}$ and $w_{ij} = 1/N_1 N_2\ \forall i, j$.

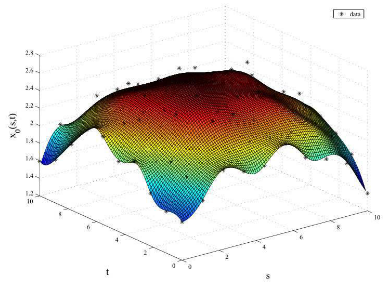
The results are shown in Figure 3, where the data points (u_i, v_j, d_{ij}) are shown by asterisks (*), and the designed spline surface $x(s,t)$ are plotted in Figure 3 (a). Figure 3 (b) shows an optimal smoothing spline $x_0(s,t)$ obtained without any constraints in (51). In addition, the corresponding derivatives $x^{(2,0)}(s,t)$ and $x_0^{(2,0)}(s,t)$ are plotted in Figure 4. We observe that the desired results are obtained by including the constraints on second partial derivative.

V. Concluding Remarks

We considered the problem of designing optimal smoothing spline surface with constraints on its derivatives. The

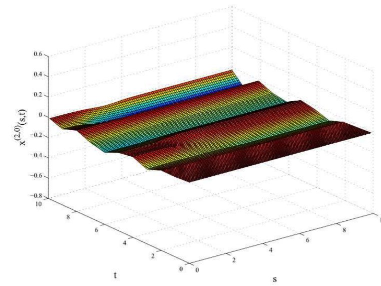


(a) Constrained case : $x(s,t)$

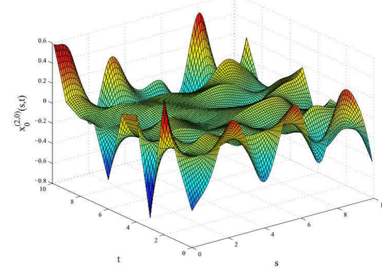


(b) Unconstrained case : $x_0(s,t)$

Fig. 3. Data points (*), (a) constrained and (b) unconstrained smoothing spline surfaces $x(s,t)$ and $x_0(s,t)$.



(a) Constrained case : $x^{(2,0)}(s,t)$



(b) Unconstrained case : $x_0^{(2,0)}(s,t)$

Fig. 4. Corresponding derivatives (a) $x^{(2,0)}(s,t)$ and (b) $x_0^{(2,0)}(s,t)$ of smoothing spline surfaces.

splines are constructed by using normalized uniform B-splines as the basis functions, hence the central issue is to determine the matrix τ consisting of optimal control points. The partial derivative $x^{(l_1,l_2)}(s,t)$ of spline surface $x(s,t)$ of degree k is expressed by using bivariate B-splines of degrees $k-l_1$ in s and $k-l_2$ in t. Then, the computation of control points $\phi_{i,j}$ are obtained as l_1-th and l_2-th backward differences of original control points $\tau_{i,j}$ in i and j respectively. This enabled us to treat systematically the problem with equality and inequality constraints over some regions on derivatives of arbitrary degree. This includes monotone and convex spline surfaces. In addition, pointwise constraints can readily be incorporated in this scheme. We demonstrated the effectiveness of design method by numerical examples of approximating monotone and concave functions. We used MATLAB for numerical computations, in particular, its function 'quadprog' for quadratic programming problems. The computational process was stable in the sense that the results did not change much for different data noise sequences. It might be possible that the shape preserving constraints as used in the examples suppress the data noises resulting in more stable construction of surfaces.

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