TWO-DIMENSIONAL POSITIVE SPLINE SMOOTHING AND ITS APPLICATION TO PROBABILITY DENSITY ESTIMATION

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ABSTRACT

Spline is a piecewise polynomial and has been widely used for interpolation and smoothing of observed data. In this paper, with the use of the sufficient condition, derived by Heß and Schmidt, for the nonnegativity of bivariate splines on square grid, we propose two-dimensional positive spline interpolation/smoothing on square grid for estimation of positive continuous functions. Moreover, we newly derive a sufficient condition for the nonnegativity on triangular grid and propose positive spline interpolation/smoothing on triangular grid. Then we estimate a two-dimensional probability density function (PDF) from its histogram by using the idea of the positive spline smoothing. Numerical experiments show the effectiveness of the newly derived sufficient condition and the proposed PDF estimator.

Index Terms—Bivariate spline, two-dimensional positive spline interpolation/smoothing, quadratic programming, density estimation.

1. INTRODUCTION

Spline is a function in a class of piecewise polynomials and has been widely used for design of continuous models in many signal and image processing applications [1], e.g., super-resolution [2], [3], computer aided design [4], [5], and regression analysis [6], [7], due to its flexibility and optimality (see, e.g., Fact 1). On the other hand, design of positive continuous functions such as probability density function (PDF) [8], [9] and power spectral density [10], [11] are also required in many applications, e.g., pattern recognition [12], [13], quantization [14], filtering [15], data analysis [16], speech enhancement [17], speech recognition [18] and sound source separation [19]. However spline interpolation and smoothing have been hardly applicable to the design of positive functions, and *logspline* has been used instead of spline [20], [21]. This is because the nonnegativity of splines is not guaranteed in general as shown in [22].

In our previous work [23], by using the sufficient condition [24] for the nonnegativity of univariate splines, we proposed one-dimensional positive spline smoothing and its application to PDF estimation. However, trying to extend this results to higher dimensions, we encounter nonobvious questions even in two-dimensional case, e.g., which grids are suitable for defining bivariate splines and which functionals are suitable as cost of optimization problems.

In this paper, as an extension of [23], we propose two-dimensional positive spline smoothing and its application to PDF estimation. In Section 2, as preliminaries, we introduce two kinds of bivariate spline spaces using square grid or triangular grid (Section 2.1), and define two-dimensional positive spline interpolation and smoothing as optimization problems (Section 2.2). In Section 3, on the basis of the derivation of the sufficient condition [24] for the nonnegativity of bivariate splines over squares (Section 3.1), we newly derive a sufficient condition for the nonnegativity over triangles (Section 3.2). Then we solve the optimization problems under the sufficient condition as quadratic programming problems (Section 3.3). Moreover, by modifying the idea of the positive spline smoothing, we estimate a two-dimensional PDF from its histogram with the use of bivariate splines (Section 3.4). In Section 4, first we numerically evaluate the effectiveness of the newly derived sufficient condition by experiments for the positive spline interpolation/smoothing (Section 4.1). Second we show the effectiveness of the proposed PDF estimator compared with the kernel density estimation [8], [9], which has been widely used for nonparametric PDF estimation, by experiments for a Gaussian mixture (Section 4.2). In Section 5, we conclude this paper.

2. PRELIMINARIES

Let $\mathbb{R}$, $\mathbb{R}_+$ and $\mathbb{Z}_+$ be respectively the set of all real numbers, nonnegative real numbers and nonnegative integers. Boldface small and capital letters respectively express a vector and a matrix. The norm of $\boldsymbol{x} := (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n$ is defined as $\|\boldsymbol{x}\| := \sqrt{\sum_{i=1}^n x_i^2}$.

2.1. Bivariate Spline Spaces

Let $\square_{n,m} := \{\mathcal{R}_{i,j} := [x_{i-1}, x_i] \times [y_{j-1}, y_j]\}_{j=1,2,\ldots,m}^{i=1,2,\ldots,n}$ be a set of all squares $R_{i,j}$ on $\Omega := [x_0, x_n] \times [y_0, y_m] \subset \mathbb{R}^2$ s.t. $x_i - x_{i-1} = 1$ for all $i = 1, 2, \ldots, n$ and $y_j - y_{j-1} = 1$ for all $j = 1, 2, \ldots, m$. For two nonnegative integers ρ and d s.t. $0 \le \rho < d$, define

$$\mathcal{S}_d^\rho(\square_{n,m}) := \{f \in C_\rho^{2\rho}(\Omega) \mid \forall \mathcal{R}_{i,j} \in \square_{n,m} \quad f|_{\mathcal{R}_{i,j}} \in \mathbb{P}_{d,d}\}$$

as the set of all bisplines of degree d and smoothness ρ on $\square_{n,m}$, where $C_\rho^{2\rho}(\Omega)$ stands for the set of all continuous functions $f : \Omega \to \mathbb{R}$ whose partial derivatives $\frac{\partial^{i+j} f}{\partial x^i \partial y^j}$ $(i, j = 0, 1, \ldots, \rho)$ are also continuous over Ω, $f|_{\mathcal{R}_{i,j}} : \mathcal{R}_{i,j} \to \mathbb{R}$ denotes the restriction of f to $\mathcal{R}_{i,j}$, and $\mathbb{P}_{d,d}$ is the set of all bivariate polynomials whose degree is d at most with regard to each variable, i.e., $\mathbb{P}_{d,d} := \{f : \mathbb{R}^2 \to \mathbb{R} : (x, y) \mapsto \sum_{p=0}^d \sum_{q=0}^d c_{p,q} x^p y^q \mid c_{p,q} \in \mathbb{R}\}$.

Assume that we observe samples of a twice continuously differentiable function $g : \Omega \to \mathbb{R}$ with additive noise $\epsilon_{i,j} \in \mathbb{R}$ at (x_i, y_j), i.e., we observe $z_{i,j} := g(x_i, y_j) + \epsilon_{i,j}$ $(i = 0, 1, \ldots, n$ and $j = 0, 1, \ldots, m)$. In this situation, a natural[1] bicubic spline $f \in \mathcal{S}_3^2(\square_{n,m})$ is often used to approximate g because it guarantees the optimality shown in the following fact [25], [26].

Fact 1 (Bicubic spline as a unique solution of a variational problem) *There always exists a unique minimizer $f^* \in C_2^4(\Omega)$ of*

$$\sum_{i=0}^n \sum_{j=0}^m |f(x_i, y_j) - z_{i,j}|^2 + \lambda \iint_\Omega \left| \frac{\partial^4 f}{\partial x^2 \partial y^2} \right|^2 \mathrm{d}x\mathrm{d}y$$

and it is a natural bicubic spline $f^* \in \mathcal{S}_3^2(\square_{n,m})$, where $\lambda > 0$ controls the trade-off between data fidelity and smoothness.

[1]A bicubic spline $f \in \mathcal{S}_3^2(\square_{n,m})$ is *natural* if $\frac{\partial^2 f}{\partial x^2}(x, y) = 0$ $\forall (x, y) \in \{x_0, x_n\} \times [y_0, y_m]$ and $\frac{\partial^2 f}{\partial y^2}(x, y) = 0$ $\forall (x, y) \in [x_0, x_n] \times \{y_0, y_m\}$.

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In order to achieve more flexibility with respect to the resolution of the discretization in Ω, partitioning of Ω into triangles has been studied [27]–[31]. Define a triangle $\mathcal{T}$ on $\mathbb{R}^2$, by specifying three vertices $\boldsymbol{v}_k := (x_k, y_k) \in \mathbb{R}^2$ $(k = 1, 2, 3)$ which are not arranged linearly, i.e., $x_1y_2 - y_1x_2 + x_2y_3 - y_2x_3 + x_3y_1 - y_3x_1 \neq 0$, as

$$\mathcal{T} := \langle \boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3 \rangle := \left\{ r\boldsymbol{v}_1 + s\boldsymbol{v}_2 + t\boldsymbol{v}_3 \in \mathbb{R}^2 \;\middle|\; \begin{array}{l} r, s, t \in [0, 1] \\ r + s + t = 1 \end{array} \right\}.$$

Then create four kinds of triangles

$$\left.\begin{array}{l} \mathcal{T}_{i,j,1} := \langle (x_{i-1}, y_{j-1}), (x_i, y_{j-1}), (\frac{x_{i-1}+x_i}{2}, \frac{y_{j-1}+y_j}{2}) \rangle \\ \mathcal{T}_{i,j,2} := \langle (x_{i-1}, y_j), (x_{i-1}, y_{j-1}), (\frac{x_{i-1}+x_i}{2}, \frac{y_{j-1}+y_j}{2}) \rangle \\ \mathcal{T}_{i,j,3} := \langle (x_i, y_j), (x_{i-1}, y_j), (\frac{x_{i-1}+x_i}{2}, \frac{y_{j-1}+y_j}{2}) \rangle \\ \mathcal{T}_{i,j,4} := \langle (x_i, y_{j-1}), (x_i, y_j), (\frac{x_{i-1}+x_i}{2}, \frac{y_{j-1}+y_j}{2}) \rangle \end{array}\right\}$$

by diagonally cutting every square $\mathcal{R}_{i,j} = [x_{i-1}, x_i] \times [y_{j-1}, y_j]$. Let $\boxtimes_{n,m} := \{\mathcal{T}_{i,j,1}, \mathcal{T}_{i,j,2}, \mathcal{T}_{i,j,3}, \mathcal{T}_{i,j,4}\}_{j=1,2,\ldots,m}^{i=1,2,\ldots,n}$ be a set of all triangles $\mathcal{T}_{i,j,k}$ on Ω. For $\rho, d \in \mathbb{Z}_+$ s.t. $0 \leq \rho < d$, define

$$\mathcal{S}_d^\rho(\boxtimes_{n,m}) := \{ f \in C^\rho(\Omega) \,|\, \forall \mathcal{T}_{i,j,k} \in \boxtimes_{n,m} \quad f|_{\mathcal{T}_{i,j,k}} \in \mathbb{P}_d \}$$

as the set of all bivariate splines of degree d and smoothness ρ on $\boxtimes_{n,m}$, where $C^\rho(\Omega)$ stands for the set of all ρ-times continuously differentiable functions over Ω, and $\mathbb{P}_d$ is the set of all bivariate polynomials whose degree is d at most, i.e., $\mathbb{P}_d := \{f : \mathbb{R}^2 \to \mathbb{R} : (x, y) \mapsto \sum_{p=0}^{d} \sum_{q=0}^{d-p} c_{p,q} x^p y^q \,|\, c_{p,q} \in \mathbb{R}\}$.

Remark 1 *For the above function spaces, $C^{2\rho}(\Omega) \subset C_\rho^{2\rho}(\Omega) \subset C^\rho(\Omega)$, $\mathbb{P}_d \subset \mathbb{P}_{d,d} \subset \mathbb{P}_{2d}$, and $\mathcal{S}_d^\rho(\square_{n,m}) \subset \mathcal{S}_{2d}^\rho(\boxtimes_{n,m})$ hold.*

2.2. Two-Dimensional Positive Spline Interpolation/Smoothing

The problem of our interest is to estimate a nonnegative function $g : \Omega \to \mathbb{R}_+$ from its nonnegative samples $z_{i,j} := g(x_i, y_j) + \epsilon_{i,j} \geq 0$. In [24], Heß and Schmidt considered the positive C^2-bispline interpolation and shown that the lowest degree is $d = 4$ for guaranteeing the existence of $f \in \mathcal{S}_d^2(\square_{n,m})$ satisfying $f(x_i, y_j) = z_{i,j}$ $(i = 0, 1, \ldots, n$ and $j = 0, 1, \ldots, m)$ and $f(x, y) \geq 0$ for all $(x, y) \in \Omega$. However, they did not show which functionals are suitable as cost of optimization problems. As an extension of the energy of local variation $\int |f''(x)|^2 \,\mathrm{d}x$ used in [23], we employ not $\iint_\Omega |\frac{\partial^4 f}{\partial x^2 \partial y^2}|^2 \,\mathrm{d}x\mathrm{d}y$ in Fact 1 but $\iint_\Omega [|\frac{\partial^2 f}{\partial x^2}|^2 + 2|\frac{\partial^2 f}{\partial x \partial y}|^2 + |\frac{\partial^2 f}{\partial y^2}|^2] \,\mathrm{d}x\mathrm{d}y$ in accordance with [29]. As a result, we consider the following two problems.

Problem 1 (Two-dimensional positive spline interpolation ($d \geq 4$)) *Find $f^* \in \mathcal{S}_d^2(\square_{n,m})$ (or $f^* \in \mathcal{S}_d^2(\boxtimes_{n,m})$) minimizing*

$$\iint_\Omega \left[\left| \frac{\partial^2 f}{\partial x^2} \right|^2 + 2 \left| \frac{\partial^2 f}{\partial x \partial y} \right|^2 + \left| \frac{\partial^2 f}{\partial y^2} \right|^2 \right] \mathrm{d}x\mathrm{d}y$$

subject to $f(x_i, y_j) = z_{i,j}$ ($i = 0, 1, \ldots, n$ and $j = 0, 1, \ldots, m$) and $f(x, y) \geq 0$ for all $(x, y) \in \Omega$.

Problem 2 (Two-dimensional positive spline smoothing ($d \geq 4$)) *Find $f^* \in \mathcal{S}_d^2(\square_{n,m})$ (or $f^* \in \mathcal{S}_d^2(\boxtimes_{n,m})$) minimizing*

$$\sum_{i=0}^{n} \sum_{j=0}^{m} |f(x_i, y_j) - z_{i,j}|^2 + \lambda \iint_\Omega \left[\left| \frac{\partial^2 f}{\partial x^2} \right|^2 + 2 \left| \frac{\partial^2 f}{\partial x \partial y} \right|^2 + \left| \frac{\partial^2 f}{\partial y^2} \right|^2 \right] \mathrm{d}x\mathrm{d}y$$

subject to $f(x, y) \geq 0$ for all $(x, y) \in \Omega$, where $\lambda > 0$.

In the next section, in order to solve the above problems, we use the sufficient condition for the nonnegativity of $f \in \mathcal{S}_d^2(\square_{n,m})$ in [24]. Moreover, on the basis of the derivation in [24], we newly derive a sufficient condition for the nonnegativity of $f \in \mathcal{S}_d^2(\boxtimes_{n,m})$.

3. POSITIVE SPLINE SMOOTHING UNDER SUFFICIENT CONDITION AND ITS EXTENSION TO PDF ESTIMATION

3.1. Sufficient Condition for The Nonnegativity over Squares

To summarize the discussion in [24], the sufficient condition for the nonnegativity of $f \in \mathcal{S}_d^2(\square_{n,m})$ over Ω was derived as follows. Suppose that a bispline $f \in \mathcal{S}_d^2(\square_{n,m})$ is expressed, over $\mathcal{R}_{i,j}$, as

$$f(x, y) = \sum_{p=0}^{d} \sum_{q=0}^{d} c_{p,q}^{i,j} s^p t^q, \tag{1}$$

where $c_{p,q}^{i,j} \in \mathbb{R}$, $s := x - x_{i-1} \in [0, 1]$ and $t := y - y_{j-1} \in [0, 1]$. Substitute $s = \frac{\alpha}{1+\alpha}$ and $t = \frac{\beta}{1+\beta}$, which imply that $s, t \in [0, 1]$ if and only if $\alpha, \beta \in \mathbb{R}_+ \cup \{\infty\} =: [0, \infty]$. After some algebra, we can obtain vectors $\boldsymbol{g}_{p,q} \in \mathbb{Z}_+^{(d+1)^2}$ $(p, q = 0, 1, \ldots, d)$ satisfying

$$(1 + \alpha)^d (1 + \beta)^d f(x, y) = \sum_{p=0}^{d} \sum_{q=0}^{d} \boldsymbol{g}_{p,q}^T \boldsymbol{c}_{i,j} \alpha^p \beta^q,$$

where $\boldsymbol{c}_{i,j} = (c_{d,d}^{i,j}, c_{d,d-1}^{i,j}, \ldots, c_{d,0}^{i,j}, c_{d-1,d}^{i,j}, \ldots, c_{0,0}^{i,j})^T \in \mathbb{R}^{(d+1)^2}$. From $(1 + \alpha)^d (1 + \beta)^d \geq 1$ and $\alpha^p \beta^q \geq 0$ for all $\alpha, \beta \in [0, \infty]$, the sufficient condition for the nonnegativity of f in (1) is

$$\boldsymbol{g}_{p,q}^T \boldsymbol{c}_{i,j} \geq 0 \quad \text{for all } i, j, p \text{ and } q. \tag{2}$$

Therefore, we can create a matrix $\boldsymbol{G}$ s.t. $\boldsymbol{Gc} \geq \boldsymbol{0} \Rightarrow f(x, y) \geq 0$ for all $(x, y) \in \Omega$, where $\boldsymbol{c} := (\boldsymbol{c}_{1,1}^T, \boldsymbol{c}_{1,2}^T, \ldots, \boldsymbol{c}_{n,m}^T)^T \in \mathbb{R}^{(d+1)^2 mn}$.

3.2. Sufficient Condition for The Nonnegativity over Triangles

By utilizing the above discussion, we newly derive a sufficient condition for the nonnegativity of $f \in \mathcal{S}_d^2(\boxtimes_{n,m})$ over Ω. Suppose that a bivariate spline $f \in \mathcal{S}_d^2(\boxtimes_{n,m})$ is expressed, over $\mathcal{T}_{i,j,k}$, as

$$f(x, y) = \sum_{p=0}^{d} \sum_{q=0}^{p} c_{p(p+1)/2+q+1}^{i,j,k} \frac{d!\, r^{d-p} s^{p-q} t^q}{(d-p)!(p-q)!q!}, \tag{3}$$

where $c_{p(p+1)/2+q+1}^{i,j,k} \in \mathbb{R}$ and $(r, s, t) \in [0, 1]^3$ $(r + s + t = 1)$ is called *barycentric coordinate* of (x, y) with respect to $\mathcal{T}_{i,j,k}$ [27], [28], e.g., the barycentric coordinate with respect to $\mathcal{T}_{i,j,1}$ is

$$(r, s, t) = (x_{i-1} - x + y_j - y, x - x_{i-1} + y_{j-1} - y, 2y - 2y_{j-1}).$$

Substitute $r = \frac{\alpha}{1+\alpha}$, $s = \frac{\beta}{1+\beta}$, and $t = 1 - r - s = \frac{1-\alpha\beta}{(1+\alpha)(1+\beta)}$, which imply that $r, s, t \in [0, 1]$ if and only if $\alpha, \beta \in [0, \infty]$ and $\alpha\beta =: \chi \in [0, 1]$. Then, we have

$$(1 + \alpha)^d (1 + \beta)^d f(x, y) = c_1^{i,j,k} \alpha^d + c_{d(d+1)/2+1}^{i,j,k} \beta^d + \sum_{p=1}^{d-1} P_{d-p}^{i,j,k}(\chi) \alpha^p + \sum_{q=1}^{d-1} Q_{d-q}^{i,j,k}(\chi) \beta^q + R_d^{i,j,k}(\chi),$$

where $P_{d-p}^{i,j,k}(\chi)$, $Q_{d-q}^{i,j,k}(\chi)$ and $R_d^{i,j,k}(\chi)$ are univariate polynomials of degree $(d - p)$, $(d - q)$ and d, respectively. For example, for $d = 4$, $P_{4-p}^{i,j,k}(\chi)$, $Q_{4-q}^{i,j,k}(\chi)$ and $R_4^{i,j,k}(\chi)$ are defined by (5) where the indices i, j and k are omitted for simplicity. Therefore, the sufficient condition for the nonnegativity of f in (3) is

$$\begin{array}{l} c_1^{i,j,k} \geq 0, \; c_{d(d+1)/2+1}^{i,j,k} \geq 0, \; P_{d-p}^{i,j,k}(\chi) \geq 0, \; Q_{d-q}^{i,j,k}(\chi) \geq 0 \\ \text{and } R_d^{i,j,k}(\chi) \geq 0 \qquad \text{for all } i, j, k, p, q \text{ and } \chi \in [0, 1]. \end{array} \tag{4}$$

Finally, by substituting $\chi := \frac{\gamma}{1+\gamma}$ and computing the coefficients of γ^δ $(\delta = 0, 1, \ldots, d)$ in $(1 + \gamma)^{d-p} P_{d-p}^{i,j,k}(\chi)$, $(1 + \gamma)^{d-q} Q_{d-q}^{i,j,k}(\chi)$ and $(1 + \gamma)^d R_d^{i,j,k}(\chi)$, we can create a matrix $\boldsymbol{G}$ s.t. $\boldsymbol{Gc} \geq \boldsymbol{0} \Rightarrow f(x, y) \geq 0$ for all $(x, y) \in \Omega$, where $\boldsymbol{c}$ is defined, with the use of $\boldsymbol{c}_{i,j,k} := (c_1^{i,j,k}, c_2^{i,j,k}, \ldots, c_{(d+1)(d+2)/2}^{i,j,k})^T \in \mathbb{R}^{(d+1)(d+2)/2}$, as $\boldsymbol{c} := (\boldsymbol{c}_{1,1,1}^T, \boldsymbol{c}_{1,1,2}^T, \ldots, \boldsymbol{c}_{n,m,4}^T)^T \in \mathbb{R}^{2(d+1)(d+2)mn}$.

3.3. Problem 1 and Problem 2 under The Sufficient Condition

In Problem 1, the cost $\iint_\Omega [|\frac{\partial^2 f}{\partial x^2}|^2 + 2|\frac{\partial^2 f}{\partial x \partial y}|^2 + |\frac{\partial^2 f}{\partial y^2}|^2] \,\mathrm{d}x\mathrm{d}y$ can be written by a quadratic form $\boldsymbol{c}^T \boldsymbol{Q} \boldsymbol{c}$, where $\boldsymbol{c}$ is the coefficient vector of $f \in \mathcal{S}_d^2(\Box_{n,m})$ (or $f \in \mathcal{S}_d^2(\boxtimes_{n,m})$) in Section 3.1 (or 3.2) and $\boldsymbol{Q}$ is a symmetric positive semidefinite matrix [31], [32]. Moreover, the conditions $f \in C_2^4(\Omega)$ (or $f \in C^2(\Omega)$) and $f(x_i, y_j) = z_{i,j}$ ($i = 0, 1, \ldots, n$ and $j = 0, 1, \ldots, m$) are respectively expressed as $\boldsymbol{H}\boldsymbol{c} = \boldsymbol{0}$ and $\boldsymbol{\mathcal{I}}\boldsymbol{c} = \boldsymbol{z} := (z_{0,0}, z_{0,1}, \ldots, z_{n,m})^T \in \mathbb{R}^{(m+1)(n+1)}$ with the use of certain sparse matrices $\boldsymbol{H}$ and $\boldsymbol{\mathcal{I}}$ [31], [33]. Therefore under the sufficient condition $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$, based on (2) (or (4)), for the nonnegativity of f, Problems 1 and 2 are expressed as follows.

Problem 1.S (Problem 1 under the sufficient condition $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$) *Find* $\boldsymbol{c}^* \in \mathbb{R}^{(d+1)^2 mn}$ *(or* $\boldsymbol{c}^* \in \mathbb{R}^{2(d+1)(d+2)mn}$*) minimizing*

$$\boldsymbol{c}^T \boldsymbol{Q} \boldsymbol{c}$$

subject to $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$*,* $\boldsymbol{H}\boldsymbol{c} = \boldsymbol{0}$ *and* $\boldsymbol{\mathcal{I}}\boldsymbol{c} = \boldsymbol{z}$*.*

Problem 2.S (Problem 2 under the sufficient condition $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$) *Find* $\boldsymbol{c}^* \in \mathbb{R}^{(d+1)^2 mn}$ *(or* $\boldsymbol{c}^* \in \mathbb{R}^{2(d+1)(d+2)mn}$*) minimizing*

$$\|\boldsymbol{\mathcal{I}}\boldsymbol{c} - \boldsymbol{z}\|^2 + \lambda \boldsymbol{c}^T \boldsymbol{Q} \boldsymbol{c}$$

subject to $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$ *and* $\boldsymbol{H}\boldsymbol{c} = \boldsymbol{0}$*, where* $\lambda > 0$*.*

Problem 1.S and Problem 2.S are convex quadratic programming problems and can be solved in polynomial time [34]–[36].

Remark 2 *In Problems 1.S and 2.S,* $\boldsymbol{c}$*,* $\boldsymbol{G}$*,* $\boldsymbol{H}$*,* $\boldsymbol{\mathcal{I}}$*, and* $\boldsymbol{Q}$ *depend on the bivariate spline spaces* $\mathcal{S}_d^2(\Box_{n,m})$ *and* $\mathcal{S}_d^2(\boxtimes_{n,m})$*. In this paper, these dependencies are omitted for readability. Moreover, by using* $\frac{\partial^{p+q} f}{\partial x^p \partial y^q}(x_i, y_j)$ *(and* $\frac{\partial^{p+q} f}{\partial x^p \partial y^q}(\frac{x_{i-1}+x_i}{2}, \frac{y_{j-1}+y_j}{2})$*) (*$p, q = 0, 1, 2$*), instead of* $\boldsymbol{c}$*, as parameters, we can reduce the size of the problems.*

3.4. Two-Dimensional PDF Estimation by Positive Splines

In this subsection, we estimate a two-dimensional probability density function (PDF) $g : \mathbb{R}^2 \to \mathbb{R}_+$ s.t. $g \in C^2(\mathbb{R}^2)$ by extending the idea of the positive spline smoothing. In this situation, we cannot observe values of g directly but construct a histogram from observed samples which are generated from g. Hence we reconstruct the PDF g from its histogram based on the observed samples.

Let $\{(u_\ell, v_\ell)\}_{\ell=1}^L$ be samples generated from g. We create a histogram by using $\mathcal{R}_{i,j}$ (or $\mathcal{T}_{i,j,k}$) as bins s.t. $x_0 < \min\{u_\ell\}$, $x_n > \max\{u_\ell\}$, $y_0 < \min\{v_\ell\}$ and $y_m > \max\{v_\ell\}$. Then by defining $L_{i,j}$ (or $L_{i,j,k}$) as the number of (u_ℓ, v_ℓ) in $\mathcal{R}_{i,j}$ (or $\mathcal{T}_{i,j,k}$), we can expect $\iint_{\mathcal{R}_{i,j}} g \,\mathrm{d}x\mathrm{d}y \approx \frac{L_{i,j}}{L}$ (or $\iint_{\mathcal{T}_{i,j,k}} g \,\mathrm{d}x\mathrm{d}y \approx \frac{L_{i,j,k}}{L}$). Moreover, by assuming $g(x, y) = 0$ for all $(x, y) \in \mathbb{R}^2 \setminus \Omega$, i.e., $\iint_\Omega g \,\mathrm{d}x\mathrm{d}y = 1$, we try to estimate g with the use of bivariate splines through the following optimization problem.

Problem 3 (Two-dimensional PDF estimation by positive splines) *Find* $f^* \in \mathcal{S}_d^2(\Box_{n,m})$ *(or* $f^* \in \mathcal{S}_d^2(\boxtimes_{n,m})$*) minimizing*

$$\sum_{i=1}^{n} \sum_{j=1}^{m} \left| \iint_{\mathcal{R}_{i,j}} f \,\mathrm{d}x\mathrm{d}y - \frac{L_{i,j}}{L} \right|^2$$

$$\left(\textit{or } \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{4} \left| \iint_{\mathcal{T}_{i,j,k}} f \,\mathrm{d}x\mathrm{d}y - \frac{L_{i,j,k}}{L} \right|^2 \right)$$

$$+ \lambda \iint_\Omega \left[\left| \frac{\partial^2 f}{\partial x^2} \right|^2 + 2 \left| \frac{\partial^2 f}{\partial x \partial y} \right|^2 + \left| \frac{\partial^2 f}{\partial y^2} \right|^2 \right] \mathrm{d}x\mathrm{d}y$$

subject to $f(x, y) \geq 0$ *for all* $(x, y) \in \Omega$*,* $\iint_\Omega f \,\mathrm{d}x\mathrm{d}y = 1$ *and* $\frac{\partial^{p+q} f}{\partial x^p \partial y^q}(x, y) = 0$ $(p, q = 0, 1, 2)$ *for all* $(x, y) \in (\{x_0, x_n\} \times [y_0, y_m]) \cup ([x_0, x_n] \times \{y_0, y_m\})$*, where* $\lambda > 0$*.*

Remark 3 *Actually, for any histogram, we can design an optimization problem like Problem 3, but here we employ* $\mathcal{R}_{i,j}$ *(or* $\mathcal{T}_{i,j,k}$*) as bins. This is because* $\iint_{\mathcal{R}_{i,j}} f \,\mathrm{d}x\mathrm{d}y$ *(or* $\iint_{\mathcal{T}_{i,j,k}} f \,\mathrm{d}x\mathrm{d}y$*) can be easily computed by using the coefficients* $c_{p,q}^{i,j}$ *(or* $c_{p(p+1)/2+q+1}^{i,j,k}$*).*

With the use of $\boldsymbol{\zeta} := \frac{1}{L}(L_{1,1}, L_{1,2}, \ldots, L_{n,m})^T \in \mathbb{R}^{mn}$ (or $\boldsymbol{\zeta} := \frac{1}{L}(L_{1,1,1}, L_{1,1,2}, \ldots, L_{n,m,4})^T \in \mathbb{R}^{4mn}$) and certain sparse matrices $\widetilde{\boldsymbol{H}}$ and $\widetilde{\boldsymbol{\mathcal{I}}}$, Problem 3 under the sufficient condition $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$ is written as the following convex quadratic programming problem.

Problem 3.S (Problem 3 under the sufficient condition $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$) *Find* $\boldsymbol{c}^* \in \mathbb{R}^{(d+1)^2 mn}$ *(or* $\boldsymbol{c}^* \in \mathbb{R}^{2(d+1)(d+2)mn}$*) minimizing*

$$\|\widetilde{\boldsymbol{\mathcal{I}}}\boldsymbol{c} - \boldsymbol{\zeta}\|^2 + \lambda \boldsymbol{c}^T \boldsymbol{Q} \boldsymbol{c}$$

subject to $\boldsymbol{G}\boldsymbol{c} \geq \boldsymbol{0}$*,* $\widetilde{\boldsymbol{H}}\boldsymbol{c} = \boldsymbol{0}$ *and* $\boldsymbol{1}^T \widetilde{\boldsymbol{\mathcal{I}}}\boldsymbol{c} = 1$*, where* $\lambda > 0$*.*

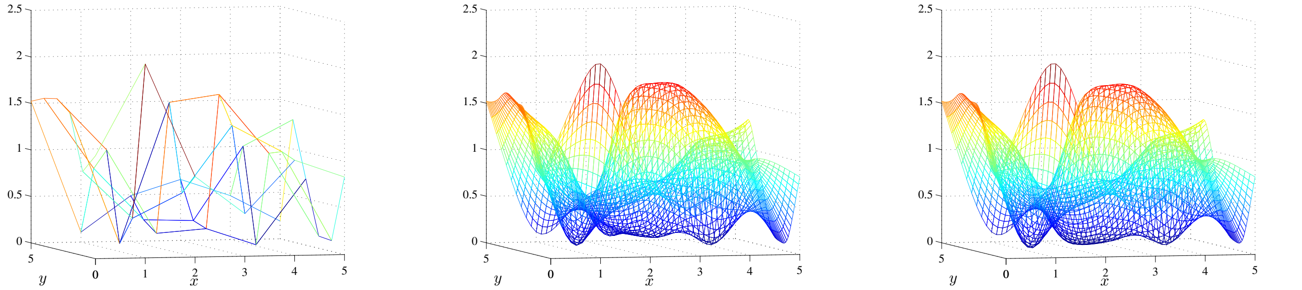
4. NUMERICAL EXPERIMENTS

4.1. Experiments for Problem 1.S and Problem 2.S

Let $\{\widetilde{z}_{i,j}\}_{j=0,1,\ldots,5}^{i=0,1,\ldots,5}$ be generated from the standard normal distribution $\mathcal{N}(0, 1)$. Define $(x_i, y_j) := (i, j)$ and $z_{i,j} := |\widetilde{z}_{i,j}|$ $(i, j = 0, 1, \ldots, 5)$. Then solve Problem 1.S and Problem 2.S with $\lambda = \frac{1}{50}, \frac{1}{250}, \frac{1}{500}$ for two bivariate spline spaces $\mathcal{S}_4^2(\Box_{5,5})$ and $\mathcal{S}_4^2(\boxtimes_{5,5})$.

Figure 1 shows an example of the results of Problem 1.S. Figures 1(a), 1(b) and 1(c) respectively depict $z_{i,j}$, $f^* \in \mathcal{S}_4^2(\Box_{5,5})$ and $f^* \in \mathcal{S}_4^2(\boxtimes_{5,5})$. In this example, the proposed sufficient condition based on (4) constructs a smoother spline in Fig. 1(c) compared with the existing condition [24] based on (2). Table 1 shows the mean values of the minimum costs of Problems 1.S and 2.S in 1000 times. From Table 1, $\mathcal{S}_4^2(\boxtimes_{5,5})$ is suitable for Problem 1.S and Problem 2.S with small λ, and $\mathcal{S}_4^2(\Box_{5,5})$ is suitable for Problem 2.S with large λ. This is because the influence of the sufficient condition is dominant for small λ, and the influence of $\mathbb{P}_d \subset \mathbb{P}_{d,d}$ is dominant for large λ.

$$\left.\begin{aligned}
P_1(\chi) &:= 4\left((c_1 + c_2 - c_3)\chi + c_3\right) \\
P_2(\chi) &:= 2\left(3(c_1 + 2c_2 - 2c_3 + c_4 - 2c_5 + c_6)\chi^2 + 2(c_2 + 3c_3 + 3c_5 - 3c_6)\chi + 3c_6\right) \\
P_3(\chi) &:= 4\left((c_1 + 3c_2 - 3c_3 + 3c_4 - 6c_5 + 3c_6 + c_7 - 3c_8 + 3c_9 - c_{10})\chi^3\right. \\
&\qquad \left. + 3(c_2 + c_3 + c_4 + c_5 - 2c_6 + c_8 - 2c_9 + c_{10})\chi^2 + 3(c_5 + c_6 + c_9 - c_{10})\chi + c_{10}\right) \\
Q_1(\chi) &:= 4\left((c_7 + c_{11} - c_{12})\chi + c_{12}\right) \\
Q_2(\chi) &:= 2\left(3(c_4 + 2c_7 - 2c_8 + c_{11} - 2c_{12} + c_{13})\chi^2 + 2(c_7 + 3c_8 + 3c_{12} - 3c_{13})\chi + 3c_{13}\right) \\
Q_3(\chi) &:= 4\left((c_2 + 3c_4 - 3c_5 + 3c_7 - 6c_8 + 3c_9 + c_{11} - 3c_{12} + 3c_{13} - c_{14})\chi^3\right. \\
&\qquad \left. + 3(c_4 + c_5 + c_7 + c_8 - 2c_9 + c_{12} - 2c_{13} + c_{14})\chi^2 + 3(c_8 + c_9 + c_{13} - c_{14})\chi + c_{14}\right) \\
R_4(\chi) &:= (c_1 + 4c_2 - 4c_3 + 6c_4 - 12c_5 + 6c_6 + 4c_7 - 12c_8 + 12c_9 - 4c_{10} + c_{11} - 4c_{12} + 6c_{13} - 4c_{14} + c_{15})\chi^4 \\
&\qquad + 4(3c_2 + c_3 + 6c_4 - 3c_5 - 3c_6 + 3c_7 - 3c_8 - 3c_9 + 3c_{10} + c_{12} - 3c_{13} + 3c_{14} - c_{15})\chi^3 \\
&\qquad + 6(c_4 + 4c_5 + c_6 + 4c_8 - 2c_9 - 2c_{10} + c_{13} - 2c_{14} + c_{15})\chi^2 + 4(3c_9 + c_{10} + c_{14} - c_{15})\chi + c_{15}
\end{aligned}\right\} \quad (5)$$

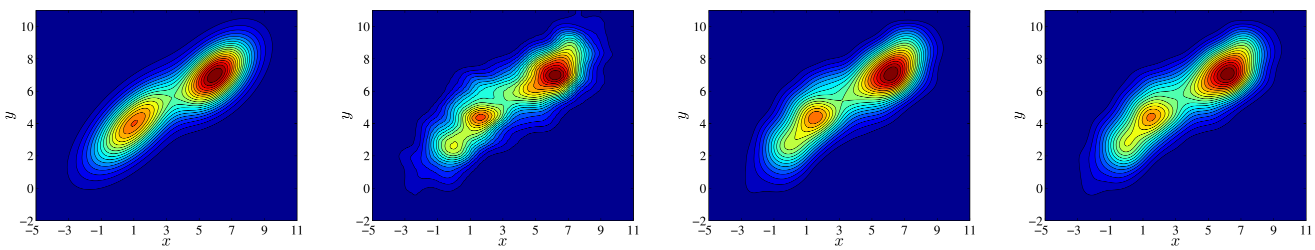


(a) $z_{i,j}$ (b) $f^* \in \mathcal{S}_4^2(\square_{5,5})$ ($\boldsymbol{c}^{*T}\boldsymbol{Q}\boldsymbol{c}^* = 148.1420$) (c) $f^* \in \mathcal{S}_4^2(\boxtimes_{5,5})$ ($\boldsymbol{c^{*T}Qc^* = 143.5709}$)

Fig. 1. Examples of the solutions $f^* \in \mathcal{S}_4^2(\square_{5,5})$ and $f^* \in \mathcal{S}_4^2(\boxtimes_{5,5})$ of Problem 1.S for $\{z_{i,j}\}_{j=0,1,\dots,5}^{i=0,1,\dots,5}$ and their costs $\boldsymbol{c}^{*T}\boldsymbol{Q}\boldsymbol{c}^*$.

Table 1. Mean values of the minimum costs $\boldsymbol{c}^{*T}\boldsymbol{Q}\boldsymbol{c}^*$ (Problem 1.S) and $\|\boldsymbol{\mathcal{I}}\boldsymbol{c}^* - \boldsymbol{z}\|^2 + \lambda\boldsymbol{c}^{*T}\boldsymbol{Q}\boldsymbol{c}^*$ (Problem 2.S) in 1000 times.

	Problem 1.S	Problem 2.S ($\lambda = \frac{1}{500}$)	Problem 2.S ($\lambda = \frac{1}{250}$)	Problem 2.S ($\lambda = \frac{1}{50}$)
$f^* \in \mathcal{S}_4^2(\square_{5,5})$	243.5967	0.442052	**0.818717**	**2.752216**
$f^* \in \mathcal{S}_4^2(\boxtimes_{5,5})$	**242.6002**	**0.440186**	0.818776	2.763259



(a) g (b) f_{KDE} ($\|g - f_{\mathrm{KDE}}\|_1 \approx 0.1402$) (c) $f^* \in \mathcal{S}_4^2(\square_{n,m})$ with $\lambda = \frac{1}{25}$ ($\|g - f^*\|_1 \approx 0.1238$) (d) $f^* \in \mathcal{S}_4^2(\boxtimes_{n,m})$ with $\lambda = \frac{1}{75}$ ($\|g - f^*\|_1 \approx \mathbf{0.1186}$)

Fig. 2. Examples of estimates f_{KDE}, $f^* \in \mathcal{S}_4^2(\square_{n,m})$ with $\lambda = \frac{1}{25}$, and $f^* \in \mathcal{S}_4^2(\boxtimes_{n,m})$ with $\lambda = \frac{1}{75}$ from $\{(u_\ell, v_\ell)\}_{\ell=1}^{1000}$ and the ℓ_1-norm errors between g and the estimates ($\|g-f\|_1 := \iint_{\mathbb{R}^2} |g - f| \,\mathrm{d}x\mathrm{d}y \approx \sum_{i=0}^{10n}\sum_{j=0}^{10m} 0.01|g(x_0+0.1i, y_0+0.1j) - f(x_0+0.1i, y_0+0.1j)|$).

Table 2. Mean values of the ℓ_1-norm errors between g and estimates f_{KDE}, $f^* \in \mathcal{S}_4^2(\square_{n,m})$ and $f^* \in \mathcal{S}_4^2(\boxtimes_{n,m})$ in 100 times.

f_{KDE} ((h_x, h_y) is based on [9])	$f^* \in \mathcal{S}_4^2(\square_{n,m})$ ($\lambda = \frac{1}{10}$ / $\mathbf{\frac{1}{25}}$ / $\frac{1}{50}$ / $\frac{1}{75}$ / $\frac{1}{100}$)	$f^* \in \mathcal{S}_4^2(\boxtimes_{n,m})$ ($\lambda = \frac{1}{10}$ / $\frac{1}{25}$ / $\frac{1}{50}$ / $\mathbf{\frac{1}{75}}$ / $\frac{1}{100}$)
0.1607	0.1634 / **0.1415** / 0.1488 / 0.1599 / 0.1696	0.2777 / 0.1849 / 0.1459 / **0.1367** / 0.1400

4.2. Experiments for Problem 3.S

Let $\{(u_\ell, v_\ell)\}_{\ell=1}^{L}$ be samples generated from a Gaussian mixture

$$g(\boldsymbol{x}) := \sum_{i=1}^{2} \frac{w_i}{2\pi\sqrt{|\boldsymbol{\Sigma}_i|}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_i)^T\boldsymbol{\Sigma}_i^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_i)},$$

where $w_1 = w_2 = 0.5$, $\boldsymbol{\mu}_1 = (1,4)^T$, $\boldsymbol{\mu}_2 = (6,7)^T$, $\boldsymbol{\Sigma}_1 = \left(\begin{smallmatrix}3&2\\2&3\end{smallmatrix}\right)$ and $\boldsymbol{\Sigma}_2 = \left(\begin{smallmatrix}2&1\\1&2\end{smallmatrix}\right)$. Define $x_0 := \lfloor\min\{u_\ell\}\rfloor$, $x_n := \lceil\max\{u_\ell\}\rceil$, $y_0 := \lfloor\min\{v_\ell\}\rfloor$ and $y_m := \lceil\max\{v_\ell\}\rceil$, where $\lfloor\cdot\rfloor$ and $\lceil\cdot\rceil$ are respectively the floor and ceiling functions. We compare the performances of Problem 3.S using $\mathcal{S}_4^2(\square_{n,m})$ and $\mathcal{S}_4^2(\boxtimes_{n,m})$ with that of the kernel density estimation [8], [9] using Gaussian kernels. The kernel density estimation constructs an estimate of g as

$$f_{\mathrm{KDE}}(x,y) = \frac{1}{L}\sum_{\ell=1}^{L}\frac{1}{2\pi h_x h_y} e^{-\left(\frac{(x-u_\ell)^2}{2h_x^2} + \frac{(y-v_\ell)^2}{2h_y^2}\right)}$$

with the use of the bandwidth $(h_x, h_y) \in \mathbb{R}_+^2$ selected by [9].

Figure 2 shows an example of the results of the proposed method and the kernel density estimation from 1000 samples $\{(u_\ell, v_\ell)\}_{\ell=1}^{1000}$. Figure 2(a) depicts the true PDF g. Figure 2(b), 2(c) and 2(d) depict the estimates f_{KDE}, $f^* \in \mathcal{S}_4^2(\square_{n,m})$ and $f^* \in \mathcal{S}_4^2(\boxtimes_{n,m})$, respectively. From Figs. 2(c) and 2(d), the proposed method constructs smoother estimates and achieves the lower ℓ_1-norm errors compared with the kernel density estimation. Table 2 shows the mean values of the ℓ_1-norm errors in 100 times. From Table 2, the proposed method using $\mathcal{S}_4^2(\boxtimes_{n,m})$ with $\lambda = \frac{1}{75}$ achieves the best performance due to more flexibilities of splines and histograms based on triangular grid.

5. CONCLUSION

In this paper, first we have newly derived a sufficient condition for the nonnegativity of $f \in \mathcal{S}_d^2(\boxtimes_{n,m})$ by utilizing the derivation of the existing sufficient condition for the nonnegativity of $f \in \mathcal{S}_d^2(\square_{n,m})$. Second we solved two-dimensional positive spline interpolation and smoothing under the sufficient condition as quadratic programming problems. Third we estimated two-dimensional PDFs as positive bivariate splines by using the idea of the positive spline smoothing. Numerical experiments show the effectiveness of the newly derived sufficient condition and the proposed PDF estimator compared with the existing condition and the kernel density estimation, respectively.

As future work, we plan to apply the positive spline smoothing to two-dimensional spectral analysis [10], [11] which is especially important in image and speech processing applications.

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