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HERMITE SCATTERED DATA FITTING BY THE PENALIZED LEAST SQUARES METHOD*

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Abstract

Given a set of scattered data with derivative values. If the data is noisy or there is an extremely large number of data, we use an extension of the penalized least squares method of von Golitschek and Schumaker [Serdica, **18** (2002), pp.1001-1020] to fit the data. We show that the extension of the penalized least squares method produces a unique spline to fit the data. Also we give the error bound for the extension method. Some numerical examples are presented to demonstrate the effectiveness of the proposed method.

Mathematics subject classification: 41A15, 65M60, 65N30.
Key words: Bivariate splines, Scattered data fitting, Extension of penalized least squares method.

1. Introduction

Suppose $V=\{v_i=(x_i,y_i)\}_{i=1}^N$ is a set of points lying in a domain $\Omega\subset\mathbf{R}^2$. Let $\{f_i^{\nu,\mu}, 0\le \nu+\mu\le r, i=1,\cdots,N\}$ be given real values. If the data is noisy or there is an extremely large number of data, it may not be appropriate to interpolate the data. This problem arises in many applications, including, e.g., surface design on airplane or car and meteorology which we will explain in our numerical examples. We will construct a function $s\in C^{r+2}(\Omega)$ which minimizes

$$P_\lambda(s):=\sum_{i=1}^N\sum_{0\le\alpha+\beta\le r}|D_x^\alpha D_y^\beta s(v_i)-f_i^{\alpha,\beta}|^2+\lambda E_r(s),$$

where $\lambda>0$ is a constant and $E_r(s)$ is the energy functional defined by

$$E_r(s)=\int_\Omega\left[\sum_{k=0}^{r+2}\binom{r+2}{k}\left[D_x^kD_y^{r+2-k}s\right]^2\right]dxdy. \tag{1.1}$$

We call this the extension of the penalized least squares method. If $W_\infty^{r+2}(\Omega)$ is the standard Sobolev space and $f_i^{\nu,\mu}=D_x^\nu D_y^\mu f(x_i,y_i)+\epsilon_i^{\nu,\mu}$ for $f\in W_\infty^{r+2}$ with noisy term $\epsilon_i^{\nu,\mu}$, we derive the error bounds for the method

$$\|f-s\|_{\infty,\Omega}\le C_1|\triangle|^{r+2}|f|_{r+2,\infty,\Omega}+C_2\lambda\|f\|_{\infty,\Omega},$$

where $|f|_{r+2,\infty,\Omega}$ denotes the maximum norm of the $(r+2)$nd derivative of f over Ω and $\|f\|_{\infty,\Omega}$ is the standard infinite norm. Here $|\triangle|$ is the size of the triangulation $\triangle$ which will be

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defined latter. For $r = 0$, this approach reduces to a typical penalized least squares problem (see, e.g., [5]). In [5], the error bound of the penalized least squares method is provided. We will generalize that result to Hermite data setting. For $r \geq 1$, the problem has received less attention. It is easy to see that when $\lambda \gg 1$, the surface is close to the energy minimization method and when $\lambda \ll 1$, the surface is close to the discrete least squares fitting. Consequently, we can choose an appropriate weight λ for our need (see, e.g., [12]).

The paper is organized as follows. In Sect. 2 we review some well-known Bernstein-Bézier notation. The extension of the penalized least squares method is explained in Sect. 3 and the existence and uniqueness are discussed there. In Sect. 4 we derive error bounds for the extension of the penalized least squares method. Finally, in last section numerical examples are presented to demonstrate the usefulness of our method.

2. Preliminaries

Given a triangulation $\triangle$ and integers $0 \leq m < d$, we write

$$S_d^m(\triangle) := \left\{ s \in C^m(\Omega) : s|_T \in P_d, \text{for all } \ T \in \triangle \right\}$$

for the usual space of splines of degree d and smoothness m, where P_d is the $\binom{d+2}{2}$ dimensional space of bivariate polynomials of degree d. Throughout the paper we shall make extensive use of the well-known Bernstein-Bézier representation of splines. For each triangle $T = \langle v_1, v_2, v_3 \rangle$ in $\triangle$ with vertices v_1, v_2, v_3, the corresponding polynomial piece $s|_T$ is written in the form

$$s|_T = \sum_{i+j+k=d} c_{ijk}^T B_{ijk}^d,$$

where B_{ijk}^d are the Bernstein-Bézier polynomials of degree d associated with T. In particular, if $(\lambda_1, \lambda_2, \lambda_3)$ is the barycentric coordinates of any point $u \in \mathbf{R}^2$ in terms of the triangle T, then

$$B_{ijk}^d(u) := \frac{d!}{i!j!k!} \lambda_1^i \lambda_2^j \lambda_3^k, \quad i + j + k = d.$$

As usual, we associate the Bernstein-Bézier coefficients $\{c_{ijk}^T\}_{i+j+k=d}$ with the domain points $\{\xi_{ijk}^T := (iv_1 + jv_2 + kv_3)/d\}_{i+j+k=d}$ and use c_ξ to denote the association.

Definition 1. *Let $\beta < \infty$. A triangulation $\triangle$ is said to be β-*quasi-uniform *provided that*

$$|\triangle| \leq \beta \rho_\triangle,$$

where $|\triangle|$ is the maximum of the diameters of the triangles in $\triangle$, and $\rho_\triangle$ is the minimum of the radii of the incircles of triangles of $\triangle$.

It is easy to see that if $\triangle$ is β-quasi-uniform, then the smallest angle in $\triangle$ is bounded below by $2/\beta$.

A determining set for a spline space $S \subseteq S_d^0(\triangle)$ is a subset $\mathcal{M}$ of the set of domain points such that if $s \in S$ and $c_\xi = 0$ for all $\xi \in \mathcal{M}$, then $c_\xi = 0$ for all domain points, i.e., $s \equiv 0$. The set $\mathcal{M}$ is called a minimal determining set (MDS) for S if there is no smaller determining set. It is known that $\mathcal{M}$ is a MDS for S if and only if every spline $s \in S$ is uniquely determined by its set of B-coefficients $\{c_\xi\}_{\xi \in \mathcal{M}}$.

Lemma 2.1. (cf. [7]) *The dual basis $\{B_\xi\}_{\xi\in\mathcal{M}}$ is a stable basis in the sense that there exist constants K_1, K_2 depending only on the smallest angle in $\triangle$ such that for all choices of the coefficient vector $\mathbf{c} = \{c_\xi\}_{\xi\in\mathcal{M}}$,*

$$K_1\|\mathbf{c}\|_\infty \le \left|\sum_{\xi\in\mathcal{M}} c_\xi B_\xi\right|_\infty \le K_2\|\mathbf{c}\|_\infty.$$

Recall from [1,2] that for any given function $f \in L_1(\Omega)$, there exists a quasi-interpolatory operator Q mapping $f \in L_1(\Omega)$ to $S_d^r(\triangle)$ with $d \ge 3r+2$, which achieves the optimal approximation order of $S_d^r(\triangle)$. The results are summarized below.

Lemma 2.2. (cf. [2]) *Let $r \ge 1$ and $d \ge 3r+2$. Suppose $f \in C^m(\Omega)$ with $m \ge 2r$. Then there exists a spline function $Q_f \in S_d^r(\triangle)$ satisfied*

$$\|D_x^\alpha D_y^\beta (f - Q_f)\|_{L_\infty(\Omega)} \le K|\triangle|^{m-\alpha-\beta}|f|_{m,\infty,\Omega}$$

for $0 \le \alpha+\beta \le m$, where $|\triangle|$ is the mesh size of $\triangle$, and $|f|_{m,\infty,\Omega}$ is the usual maximum norm of the derivatives of order m of f over Ω.

When $d < 3r+2$, similar approximation results are available for some special spline spaces, see, e.g., [6,8–11].

3. Existence and Uniqueness of Solutions to the Extension Method

Consider a spline space $S = S_d^{r+2}(\triangle)$ with $d \ge 3r+8$. Note that using the locally supported basis functions (cf. [3]), any spline function s in the space can be represented by $s = \sum_{i=1}^M c_i\phi_i$, for some set of coefficients $\{c_i\}_{i=1}^M$.

The extension of penalized least squares method is to find $s_{\lambda,f} \in S$ such that

$$P_\lambda(s_{\lambda,f}) = \min\{P_\lambda(s) : s \in S\}, \tag{3.1}$$

where $\lambda > 0$ is a positive weight,

$$P_\lambda(s) := \sum_{i=1}^N \sum_{0\le\alpha+\beta\le r} |D_x^\alpha D_y^\beta s(v_i) - f_i^{\alpha,\beta}|^2 + \lambda E_r(s) \tag{3.2}$$

and $E_r(s)$ denote the energy functional defined by (1.1).

This section is mainly concerned with the existence and uniqueness of solution $s_{\lambda,f} \in S$ satisfying (3.1).

Theorem 3.1. *Fix a $\lambda > 0$. Suppose that all vertices of $\triangle$ are the part of the data locations. Then there exists a unique $s_{\lambda,f} \in S$ satisfying* (3.1).

Proof. It is easy to show the existence of solution. For simplicity, we omit the details here, and we just show the uniqueness of the minimizer $s_{\lambda,f}$. Suppose that we have two solutions $s_{\lambda,f}$ and $\hat{s}_{\lambda,f}$. Let $\mathbf{c}$ and $\hat{\mathbf{c}}$ be the two coefficients associated with $s_{\lambda,f}$ and $\hat{s}_{\lambda,f}$ respectively. Since P_λ is a convex functional, we have, for any $z \in [0,1]$,

$$\begin{aligned}&P_\lambda(zs_{\lambda,f} + (1-z)\hat{s}_{\lambda,f})\\ \le& zP_\lambda(s_{\lambda,f}) + (1-z)P_\lambda(\hat{s}_{\lambda,f}) = P_\lambda(s_{\lambda,f}).\end{aligned} \tag{3.3}$$

That is, $P_\lambda(zs_{\lambda,f} + (1-z)\hat{s}_{\lambda,f})$ is a constant function for $z \in [0,1]$. It follows that

$$\frac{\partial}{\partial z} P_\lambda(zs_{\lambda,f} + (1-z)\hat{s}_{\lambda,f}) = 0 \quad \text{for all } z \in [0,1].$$

Consequently,

$$\begin{aligned} 0 &= \frac{\partial}{\partial z} P_\lambda(zs_{\lambda,f} + (1-z)\hat{s}_{\lambda,f}) \\ &= 2\lambda z(\mathbf{c}-\hat{\mathbf{c}})^T K(\mathbf{c}-\hat{\mathbf{c}}) + 2z(\mathbf{c}-\hat{\mathbf{c}})^T B(\mathbf{c}-\hat{\mathbf{c}}) - 2\mathbf{b}^T(\mathbf{c}-\hat{\mathbf{c}}) \end{aligned} \tag{3.4}$$

for all $z \in [0,1]$. Since both K and B are nonnegative definite, we have

$$(\mathbf{c}-\hat{\mathbf{c}})^T K(\mathbf{c}-\hat{\mathbf{c}}) = 0 \ \text{ and } \ (\mathbf{c}-\hat{\mathbf{c}})^T B(\mathbf{c}-\hat{\mathbf{c}}) = 0. \tag{3.5}$$

The first equation is equivalent to

$$E(s_{\lambda,f} - \hat{s}_{\lambda,f}) = 0$$

which implies that $s_{\lambda,f} - \hat{s}_{\lambda,f}$ is a polynomial of degree $r+1$. The second equation in (3.5) implies that

$$D_x^\alpha D_y^\beta (s_{\lambda,f} - \hat{s}_{\lambda,f}) = 0$$

at all vertices of $\triangle$ for any $\alpha + \beta \le r$. Thus, it is easy to see that

$$s_{\lambda,f} - \hat{s}_{\lambda,f} \equiv 0.$$

Hence, the minimizer is unique. □

4. Error Bounds for the Extension Method

In this section we derive error bounds for the extension of penalized least squares method. Let X, Y and S be linear spaces of functions on $\mathbf{R}^2$ where $S \subseteq Y \subseteq X$. Suppose $\|\cdot\|_X : X \to \mathbf{R}$ and $\|\cdot\|_Y : Y \to \mathbf{R}$ are semi-norms induced by semi-definite inner products $\langle \cdot, \cdot \rangle$ on X and $[\cdot,\cdot]$ on Y respectively, where

$$\begin{aligned} \langle f, g \rangle &:= \sum_{i=1}^N \sum_{0 \le \alpha+\beta \le r} D_x^\alpha D_y^\beta f(v_i) D_x^\alpha D_y^\beta g(v_i), \\ [f,g] &:= \sum_{\tau \in \triangle} \int_\tau \left[\sum_{k=0}^{r+2} \binom{r+2}{k} \left[D_x^k D_y^{r+2-k} f D_x^k D_y^{r+2-k} g \right] \right] dxdy. \end{aligned}$$

Given $f \in X$ and $\lambda > 0$, we need to find $s_{\lambda,f} \in S$ such that

$$P_\lambda(s_{\lambda,f}) = \min_{s \in S} P_\lambda(s) \tag{4.1a}$$

where

$$P_\lambda(s) := \|f - s\|_X^2 + \lambda \|s\|_Y^2. \tag{4.1b}$$

Let us introduce a discrete least square fitting: $s_f \in S$ is called a discrete least squares fit of f if

$$\|f - s_f\|_X^2 = \min_{s \in S} \|f - s\|_X^2. \tag{4.2}$$

It is easy to see that the extension of the penalized least squares approximation $s_{\lambda,f}$ of f is characterized by

$$\langle f - s_{\lambda,f}, u\rangle = \lambda[s_{\lambda,f}, u], \qquad \forall u \in S, \tag{4.3}$$

while s_f is characterized by

$$\langle f - s_f, u\rangle = 0, \qquad \forall u \in S, \tag{4.4}$$

It follows from (4.3)-(4.4) that

$$\langle s_f - s_{\lambda,f}, u\rangle = \lambda[s_{\lambda,f}, u], \qquad \forall u \in S. \tag{4.5}$$

Lemma 4.1. *For each $f \in X$ and $\lambda > 0$, we have*

$$\|s_{\lambda,f}\|_Y \leq \|s_f\|_Y, \tag{4.6}$$

and

$$\|s_f - s_{\lambda,f}\|_X \leq \sqrt{\lambda}\|s_f\|_Y, \tag{4.7}$$

where $s_{\lambda,f}$ and s_f are defined by (4.3)-(4.4).

Proof. The proof is the same as that of Theorem 6.1 in [5]. For simplicity, we omit the details here. □

Lemma 4.2. *Suppose $X \subseteq L_\infty(\Omega)$, and let*

$$K_S := \sup\left\{\frac{\|s\|_Y}{\|s\|_X} : s \in S, s \neq 0\right\} < \infty, \tag{4.8a}$$

$$k_S := \sup\left\{\frac{\|s\|_{\infty,\Omega}}{\|s\|_X} : s \in S, s \neq 0\right\} < \infty. \tag{4.8b}$$

Then

$$\|s_f - s_{\lambda,f}\|_{\infty,\Omega} \leq \lambda k_S K_S \|s_f\|_Y \tag{4.9}$$

Proof. It follows from (4.5) and the Cauchy-Schwarz inequality that

$$\|s_f - s_{\lambda,f}\|_X^2 = \lambda[s_{\lambda,f}, s_f - s_{\lambda,f}] \leq \lambda\|s_{\lambda,f}\|_Y\|s_f - s_{\lambda,f}\|_Y.$$

By the definition of K_S and (4.6), we get

$$\|s_f - s_{\lambda,f}\|_X^2 \leq \lambda\|s_f\|_Y K_S\|s_f - s_{\lambda,f}\|_X.$$

Then using

$$\|s_f - s_{\lambda,f}\|_{\infty,\Omega} \leq k_S\|s_f - s_{\lambda,f}\|_X,$$

gives (4.9). □

Below we present our main result in the paper.

Theorem 4.1. *Suppose $\triangle$ is a β-quasi-uniform triangulation and assume that*

$$L := \sup\left\{\frac{\|s\|_X}{\|s\|_{\infty,\Omega}} : s \in S, s \neq 0\right\} < \infty. \tag{4.10}$$

Then there exist constants C_1 and C_2 depending on λ, d, M and β if Ω is convex, and also on the Lipschitz constant $L_{\partial\Omega}$ of the boundary of Ω if Ω is non-convex. Let $s_{\lambda,f}$ be the spline minimizer P_λ defined by (4.1)*. Then*

$$\|f - s_{\lambda,f}\|_{\infty,\Omega} \le C_1|\triangle|^{r+2}|f|_{r+2,\infty,\Omega} + C_2\lambda\|f\|_{\infty,\Omega} \tag{4.11}$$

for every function $f \in W^{r+2}_\infty(\Omega)$.

Proof. It follows from Lemma 4.2 and the definition of K_S that

$$\|s_f - s_{\lambda,f}\|_{\infty,\Omega} \le \lambda k_S K_S^2 \|s_f\|_X.$$

Note that

$$\|s_f\|_{\infty,\Omega} \le \|s_f - f\|_{\infty,\Omega} + \|f\|_{\infty,\Omega}.$$

Then by (4.10)

$$\begin{aligned}\|s_f - s_{\lambda,f}\|_{\infty,\Omega} &\le \lambda L k_S K_S^2 \|s_f\|_{\infty,\Omega}\\ &\le \lambda L k_S K_S^2 \Big(\|s_f - f\|_{\infty,\Omega} + \|f\|_{\infty,\Omega}\Big).\end{aligned} \tag{4.12}$$

Next by the definition of Q_f, we can see that

$$\|f - Q_f\|_X^2 = \min_{s\in S} \|f - s\|_X^2. \tag{4.13}$$

Consequently, $s_f = Q_f$. Thus using Lemma 2.2 gives

$$\|f - s_f\|_{\infty,\Omega} \le K|\triangle|^{r+2}|f|_{r+2,\infty,\Omega}.$$

Using the fact

$$\|f - s_{\lambda,f}\|_{\infty,\Omega} \le \|s_f - s_{\lambda,f}\|_{\infty,\Omega} + \|f - s_f\|_{\infty,\Omega}$$

we obtain

$$\|f - s_{\lambda,f}\|_{\infty,\Omega} \le \Big(\lambda L k_S K_S^2 + 1\Big)\|s_f - f\|_{\infty,\Omega} + \lambda L k_S K_S^2 \|f\|_{\infty,\Omega}.$$

Consequently, we have (4.11) with $C_1 = K(\lambda L k_S K_S^2 + 1)$ and $C_2 = L k_S K_S^2$. □

5. Numerical Experiments

In this section we present numerical experiments for our method.

Example 5.1 Consider 1000 random points $\{(x_i, y_i)\}$ over $[0,1]\times[0,1]$ as shown in Fig. 5.1. Let $\{(x_i, y_i, f(x_i, y_i) + \epsilon_i), i = 1, \dots, 1000\}$ be a scattered data set, where

$$\begin{aligned}f(x,y) =&0.75\exp(-0.25(9x-2)^2 - 0.25(9y-2)^2)\\ &+ 0.75\exp(-(9x+1)^2/49 - (9y+1)/10)\\ &+ 0.5\exp(-0.25(9x-7)^2 - 0.25(9y-3)^2)\\ &- 0.2\exp(-(9x-4)^2 - (9y-7)^2),\end{aligned}$$

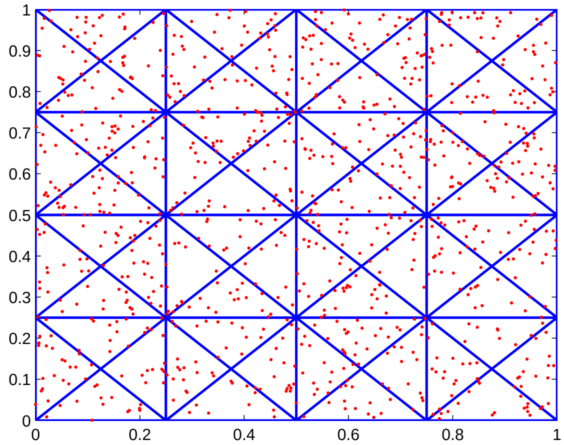

Fig. 5.1. The scattered data and the triangulation $\triangle$

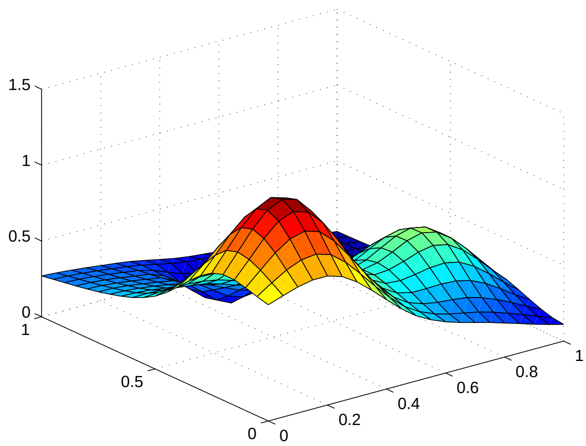

Fig. 5.2. The original Franke function

which is the well-known Franke function, (see Fig.5.2) and ϵ_i are noisy terms. We set ϵ_i to be a random number between -0.01 to 0.01. The spline spaces $S_8^2(\triangle)$ is employed to find the fitting surfaces, where $\triangle$ is the triangulation given in Fig. 5.1. Furthermore, we choose different λ to check the difference of the surface create by our method.

In Fig.(5), the surfaces created by using the extension method with $\lambda = 0.01,\ 0.1$ and 0.5 are presented. It is observed from the plots that the surface becomes less deflective when λ becomes large. So we can adjust λ to create the surface as we need.

Below, we present an example to illustrate an application of our method.

Example 5.2 We consider the reconstruction of a wind potential function. We are given a set of wind velocity measurements over 1500 places in China in one day and required to construct the wind potential function W. Let $\{(x_i, y_i, W_i^{1,0}, W_i^{0,1}, i = 1, \cdots, 1500\}$ be the given wind velocity values. In order to uniquely determine the wind potential, we assume that $W_1^{0,0} = 0$. Let $\lambda = 0.01$ and $\triangle$ be a triangulation of the part of data locations as shown in Fig. 5.4. We

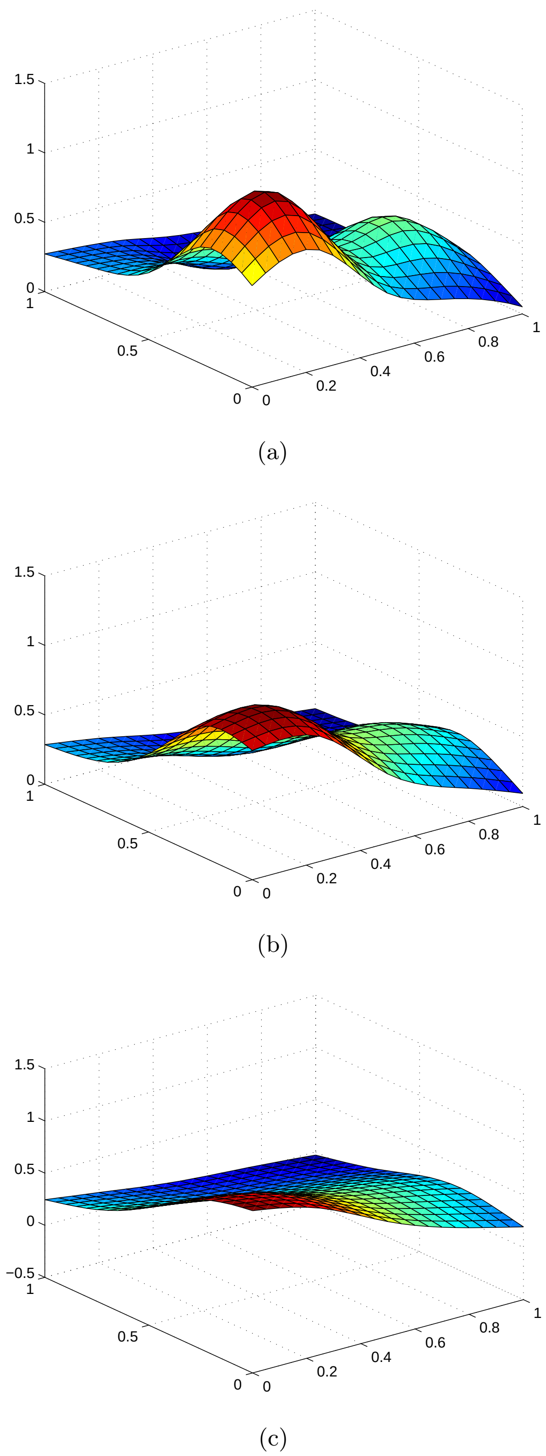

Fig. 5.3. Example 5.1: The surface created by the extension method with (a): $\lambda = 0.01$, (b): $\lambda = 0.1$ and (c): $\lambda = 0.5$

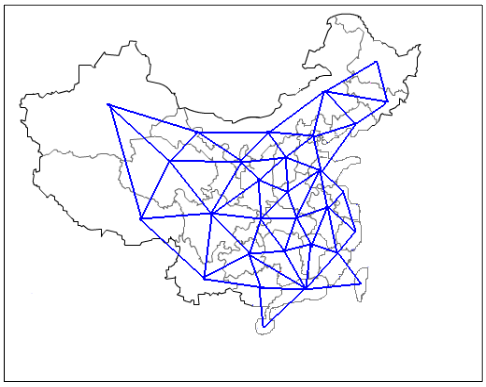

Fig. 5.4. A triangulation $\triangle$ of the data locations over China

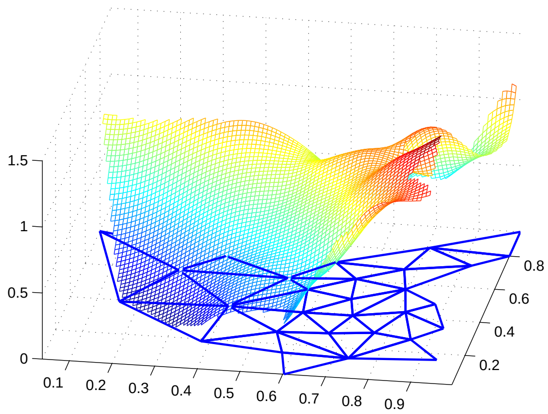

Fig. 5.5. The wind potential function

use the spline space $S_8^2(\triangle)$. We find the spline function $s_W \in S_8^2(\triangle)$ satisfying

$$P_\lambda(s_W) = \min\left[\sum_{i=1}^{1500}\sum_{\alpha+\beta=1}\left|D_x^\alpha D_y^\beta s(v_i) - W_i^{\alpha,\beta}\right|^2 + \left|s(v_1) - W_1^{0,0}\right|^2 + \lambda E_3(s)\right],$$

where

$$E_3(s) = \int_\triangle \left[\sum_{k=0}^{3}\binom{3}{k}\Big[\left(\frac{\partial}{\partial x}\right)^k\left(\frac{\partial}{\partial y}\right)^{3-k} s\Big]^2\right]dxdy.$$

In fact, we can show that there exists a unique solution s_W in any spline space $S_d^r(\triangle)$ of smoothness $r \geq 2$ and $d \geq 3r+2$. The proof is almost the same as Theorem 3.1. In Fig. 5.5, the spline reconstruction of the wind potential function is presented. The wind velocity values $\{(x_i, y_i, W_i^{1,0}, W_i^{0,1}, i = 1, \cdots, 1500\}$ are shown in Fig. 5.6.

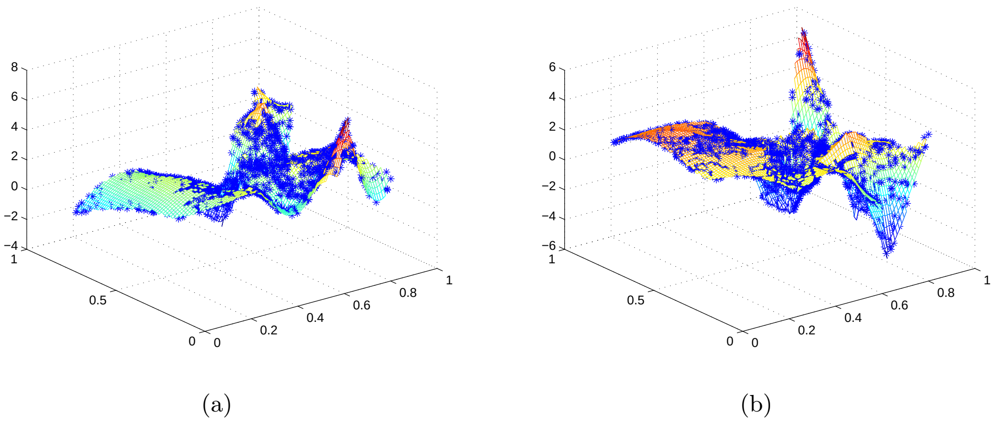

Fig. 5.6. The wind velocity in (a) x-direction, and (b): y-direction

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