Multivariate Splines for Data Fitting and Approximation

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Abstract. Methods for scattered data fitting using multivariate splines will be surveyed in this paper. Existence, uniqueness, and computational algorithms for these methods, as well as their approximation properties will be discussed. Some applications of multivariate splines for data fitting will be briefly explained. Some new research initiatives of scattered data fitting will be outlined.

§1. Introduction

Given a set of scattered data, e.g., $\{(x_i, y_i, z_i), i = 1, \cdots, N\}$, we need to find a smooth function or surface S such that

$$S(x_i, y_i) = z_i, \quad i = 1, \cdots, N,$$

if z_i are very accurate measurements or

$$S(x_i, y_i) \approx z_i, \quad i = 1, \cdots, N,$$

if z_i are subject to some random noises. Note that nowadays, N is usually very large. Three key requirements are 1) S must be a smooth surface; 2) S resembles the shape of the data; and 3) S can be efficiently computed. In this paper we explain how to use multivariate splines for solving scattered data fitting problems, and survey some recent results how well spline surfaces approximate the given data. Finally, we shall point out some new directions of research on multivariate splines for data fitting in statistics.

§2. Multivariate Splines

Let Δ be a triangulation of a domain containing $\{(x_i, y_i), i = 1, \cdots, N\}$. Define by

$$S^r_d(\Delta) = \{s \in C^r(\Omega), s|_t \in \mathbf{P}_d, t \in \Delta\}$$

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the spline space of smoothness r and degree d over Δ. Let $|\Delta|$ be the longest edge length of Δ, and ρ_Δ be the smallest inradius of triangle $t \in \Delta$. Let

$$\frac{|\Delta|}{\rho_\Delta} \le \beta < \infty.$$

Larry Schumaker and I recently wrote a monograph on multivariate splines (cf. [Lai and Schumaker'07]). The book contains all of the basics and necessary background material for this paper. Thus, I refer to the book for notation, definitions, and approximation properties of multivariate splines. In the rest of the paper, I shall discuss multivariate splines for scattered data fitting along with methods and approximation results not contained in the book.

§3. Methods for Scattered Data Fitting and Interpolation

The following methods for fitting a given set of data are available in the literature.

- Minimal Energy Method;
- Discrete Least Squares Method;
- Penalized Least Squares Spline Method;
- L_1 Spline Method;
- Least Absolute Deviation Method;
- L_1 Smoothing Spline Method;
- local or ad hoc methods, etc..

We shall give a review of these methods. We need to explain several fundamental questions concerning each method: if a method has a solution or not (i.e., the existence and uniqueness), how to compute that solution (i.e., numerical algorithms), whether the solution surface resembles the given data (i.e., approximation properties), and what to do when the amount of data is very large.

3.1. Minimal Energy Method

Let $E(f)$ be the thin-plate energy functional

$$E(f) = \int_\Omega \left(\left(\frac{\partial^2}{\partial x^2} f \right)^2 + 2 \left(\frac{\partial^2}{\partial x \partial y} f \right)^2 + \left(\frac{\partial^2}{\partial y^2} f \right)^2 \right) dxdy.$$

Let $\Lambda(f) = \{s \in S^r_d(\Delta), s(x_i, y_i) = f_i, i = 1, \cdots, N\}$. Find $S_f \in \Lambda(f)$ such that

$$E(S_f) = \min\{E(s), \quad s \in \Lambda(f)\}.$$

The following result was proved in [von Golitschek, Lai, and Schumaker'02] and in [Awanou, Lai, Wenston'06] by different methods.

Theorem 1. *If $\Lambda(f)$ is not empty, there exists a unique interpolatory spline in $S^r_d(\Delta)$.*

Once we have an interpolatory surface, we would like to know how the surface resembles the given data. Let $W^2_\infty(\Omega)$ be the Sobolev space of all functions whose second derivatives are essentially bounded over Ω. $|f|_{2,\infty,\Omega}$ is the maximal norm of all second order derivatives of f over Ω. The following results can be found in [von Golitschek, Lai, and Schumaker'02].

Theorem 2. *Suppose $z_i = f(x_i, y_i)$, $i = 1, \cdots, N$, for $f \in W^2_\infty(\Omega)$. Let $d \geq 3r + 2$, and let Δ be a triangulation of the data sites $\{(x_i, y_i), i = 1, \cdots, N\}$. Then*

$$\|s_f - f\|_{L_\infty(\Omega)} \leq C|\Delta|^2 |f|_{2,\infty,\Omega}.$$

Our next concern is how to compute interpolatory minimal energy splines using a spline space of arbitrary degree d and arbitrary smoothness r with $d \geq 3r + 2$. The following computational scheme was described in [Awanou, Lai and Wenston'06].

(1) Express each $s \in S^{-1}_d(\Delta)$ in B-form (cf. [de Boor'87]), i.e.,

$$s(x, y)|_t = \sum_{i+j+k=d} c^t_{ijk} B^{d,t}_{ijk}(x, y),$$

where $B^{d,t}_{ijk}$ are Bernstein-Bézier basis functions defined only on t. Let $\mathbf{c} = (c^t_{ijk}, i + j + k = d, t \in \Delta)$ be a coefficient vector for s.

(2) When $s \in S^r_d(\Delta)$, there are smoothness conditions over interior edges of Δ (cf. [Farin'86]). The smoothness conditions are linear. Put all smoothness conditions together to write

$$\mathcal{H}\mathbf{c} = 0,$$

for a matrix $\mathcal{H}$, i.e., $s \in S^r_d(\Delta)$ iff $\mathcal{H}\mathbf{c} = 0$.

(3) Compute the energy functional $E(s) = \mathbf{c}^T \mathcal{E} \mathbf{c}$ for an energy matrix $\mathcal{E}$ which is a diagonally block matrix.

(4) The interpolatory conditions can be written $\mathcal{I}\mathbf{c} = \mathbf{f}$ for a matrix $\mathcal{I}$ and a vector $\mathbf{f}$ containing all data values z_i.

(5) The minimal energy method for interpolatory splines is equivalent to finding $\mathbf{c}$ such that

$$\min\{\mathbf{c}^T \mathcal{E} \mathbf{c}, \text{ subject to } \mathcal{H}\mathbf{c} = 0, \mathcal{I}\mathbf{c} = \mathbf{f}\}.$$

(6) By the Lagrange multiplier method, we solve

$$\begin{bmatrix} \mathcal{E} & \mathcal{H}^T & \mathcal{I}^T \\ \mathcal{H} & 0 & 0 \\ \mathcal{I} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \mathbf{f} \end{bmatrix}.$$

(7) To solve this system, we use the following iterative method introduced in [Awanou, Lai, Wenston'06]:

$$\left(\mathcal{E} + \frac{1}{\epsilon}\begin{bmatrix}\mathcal{H}^T & \mathcal{I}^T\end{bmatrix}\begin{bmatrix}\mathcal{H}\\ \mathcal{I}\end{bmatrix}\right)\mathbf{c}^{(1)} = \frac{1}{\epsilon}\mathcal{I}^T\mathbf{f},$$

$$\left(\mathcal{E} + \frac{1}{\epsilon}\begin{bmatrix}\mathcal{H}^T & \mathcal{I}^T\end{bmatrix}\begin{bmatrix}\mathcal{H}\\ \mathcal{I}\end{bmatrix}\right)\mathbf{c}^{(k+1)} = \mathcal{E}\mathbf{c}^{(k)} + \frac{1}{\epsilon}\mathcal{I}^T\mathbf{f},$$

for $k = 1, 2, \cdots$ and $\epsilon > 0$, e.g., $\epsilon = 10^{-6}$.

We need to show that the iterative method above is convergent. To this end, recall that a matrix A is positive definite with respect to B if $\mathbf{c}^T A\mathbf{c} \geq 0$ and if $A\mathbf{c} = 0$ and $B\mathbf{c} = 0$ for some $\mathbf{c}$, then $\mathbf{c} = 0$. In [Awanou and Lai'05], we proved the following (cf. [Awanou, Lai, and Wenston'06] for a similar result).

Theorem 3. *Suppose that $\mathcal{E}$ is positive definite with respect to $[\mathcal{H}, \mathcal{I}]^T$. Then the above iteration converges, and*

$$\|\mathbf{c}^{(k+1)} - \mathbf{c}\| \leq C\epsilon^k, \quad \forall k \geq 1.$$

When the number of data sites is large, e.g., $N > 1000$, a computer may not be powerful enough to solve the linear system. A domain decomposition technique for computing an approximation of the minimal energy spline interpolation was proposed in [Lai and Schumaker'03]. The ideas of domain decomposition for scattered data fitting can be explained as follows.

Let $D_1(t)$ be the union of all triangles in Δ which share a vertex or edge with t, and $D_{k+1}(t)$ the union of all triangles sharing a vertex or edge with triangles in $D_k(t)$. For $k \geq 1$, we compute a minimal energy interpolatory spline $S_{f,t,k} \in \Lambda(f)$ such that

$$E_{D_k(t)}(S_{f,t,k}) = \min\{E_{D_k(t)}(s), s \in \Lambda(f|_t)\},$$

$$E_{D_k(t)}(s) = \int_{D_k(t)} \left(\left(\frac{\partial^2}{\partial x^2} f\right)^2 + 2\left(\frac{\partial^2}{\partial x \partial y} f\right)^2 + \left(\frac{\partial^2}{\partial y^2} f\right)^2\right).$$

The following result was established in [Lai and Schumaker'03].

Theorem 4. *Suppose that $f \in C^2(\Omega)$. For $d \geq 3r+2$, there is a $0 < \rho < 1$ such that*

$$\|S_f - S_{f,t,k}\|_{L_\infty(t)} \leq C\rho^k |f|_{2,\infty,\Omega}$$

for $k \geq 1$, where C is a constant dependent on d, β.

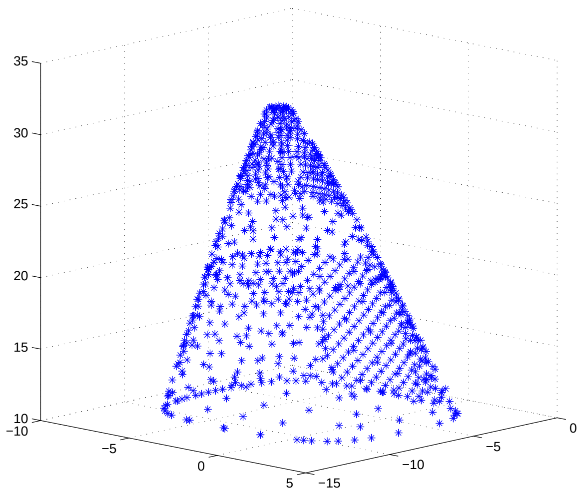

Fig. 1. A set of scattered data (courtesy Tom Grandine).

This result shows that a (global) minimal energy spline interpolation S_f can be approximated by local minimal energy spline interpolations $S_{f,t,k}$ for all $t \in \triangle$. That is, for each triangle t, one can use a local minimal energy spline interpolation $S_{f,t,k}$ to replace the global one $S_f|_t$ within some tolerance. In the following we give a numerical example.

Example 1. *We are given a set of data shaped like a cone in Fig. 1. There are about 900 points in 3D Euclidean space. A Delaunay triangulation of the given data locations is shown in Fig. 2. A piecewise linear interpolation is given in Fig. 3. We use C^1 quintic spline functions and find the minimal energy interpolatory spline surface as shown in Fig. 4. It is clear that the surface is smooth although there are a few bumpy spots which indicate imperfect data values.*

We now outline some extensions to incomplete data interpolation, Hermite data interpolation, hole filling, and spherical scattered data interpolation.

When a given data set is incomplete, i.e., values at some grid locations are not given as shown in Fig. 5, we can still use the minimal energy method with the assumption that the spline coefficients at those vertices which have no given data values are free. The computation is exactly as above. Indeed, the interpolation conditions $\mathcal{I}\mathbf{c} = \mathbf{f}$ have fewer entries than the standard one.

We use C^1 quintic spline to find an interpolatory surface using the minimal energy method. It is clear from Fig. 6 that the surface is smooth.

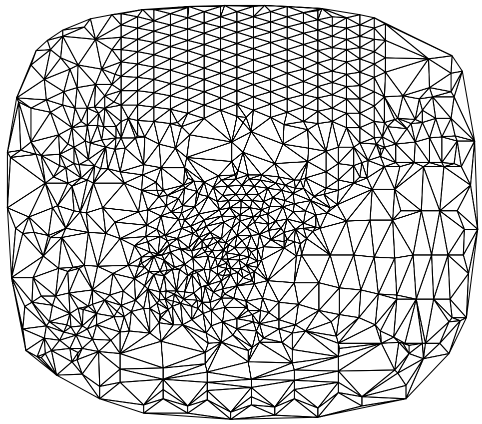

Fig. 2. A triangulation of the given data locations.

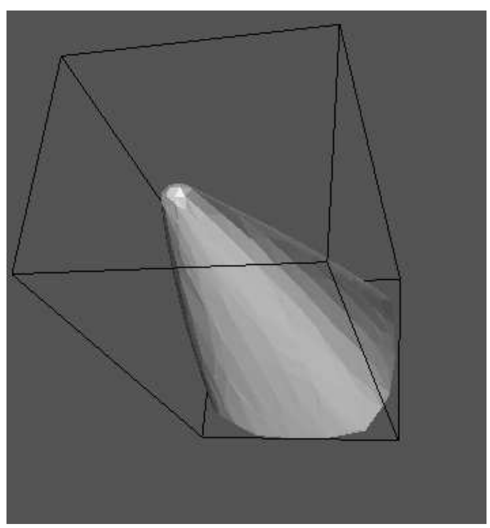

Fig. 3. A piecewise linear interpolation.

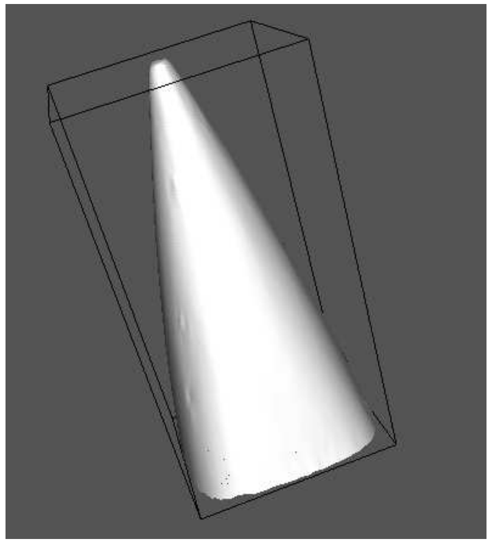

Fig. 4. A C^1 quintic spline interpolation.

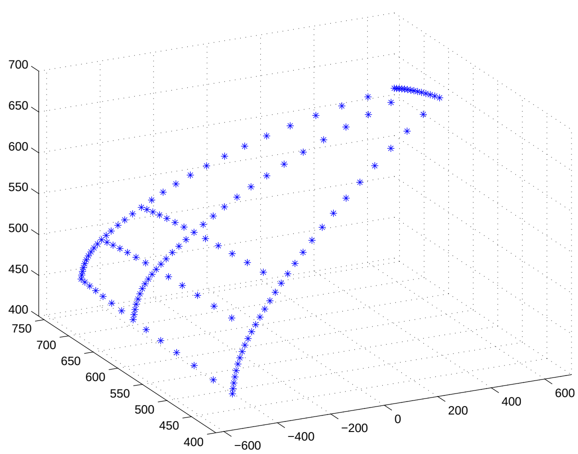

Fig. 5. A set of data points (courtesy Gerald Farin).

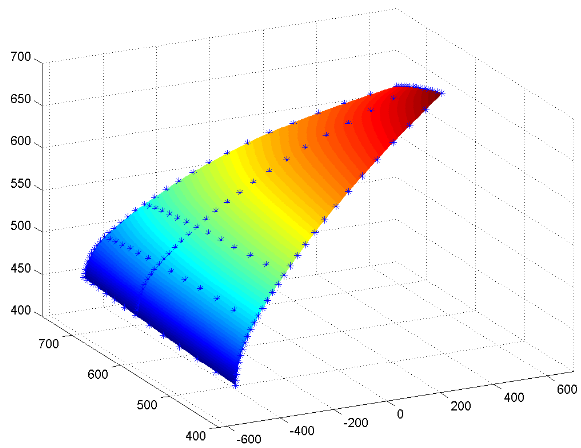

Fig. 6. A C^1 quintic spline surface with the given data locations.

When a given data set contains Hermite data values

$$\{(x_i, y_i, D^\alpha f(x_i, y_i), |\alpha| \le r, i = 1, \cdots, N\},$$

we can use the minimal energy method to find a spline function H_f in $S_d^r(\Delta)$ to interpolate all the given data values including derivatives, i.e..

$$D^\alpha H_f(x_i, y_i) = D^\alpha f(x_i, y_i), \quad |\alpha| \le r, \quad i = 1, \cdots, N.$$

The existence, uniqueness, and approximation properties of H_f have been discussed in [Zhou, Han and Lai'07].

When the given data values as well as normal derivative values are all on the boundary of a surface hole, we can use the minimal energy method to find a C^1 spline surface patch to mend the hole (cf. [Chui and Lai'00]). See the example in Fig. 7.

When the given data values are over the spherical domain, we can use the spherical splines [Alfeld, Neamtu, Schumaker'96] and the minimal energy method to find a C^r interpolatory spline surface. The framework of minimal energy interpolatory splines in the bivariate setting has been generalized to the spherical setting (cf. [Baramidze, Lai and Shum'06]). The computational algorithm is similar to the one for bivariate polynomial splines. In Fig. 8, we present a set of normalized scattered data values over the surface of the earth. They are simulated measurements from a German satellite CHAMP launched on 2000. We use C^1 quintic spherical splines to find an interpolant.

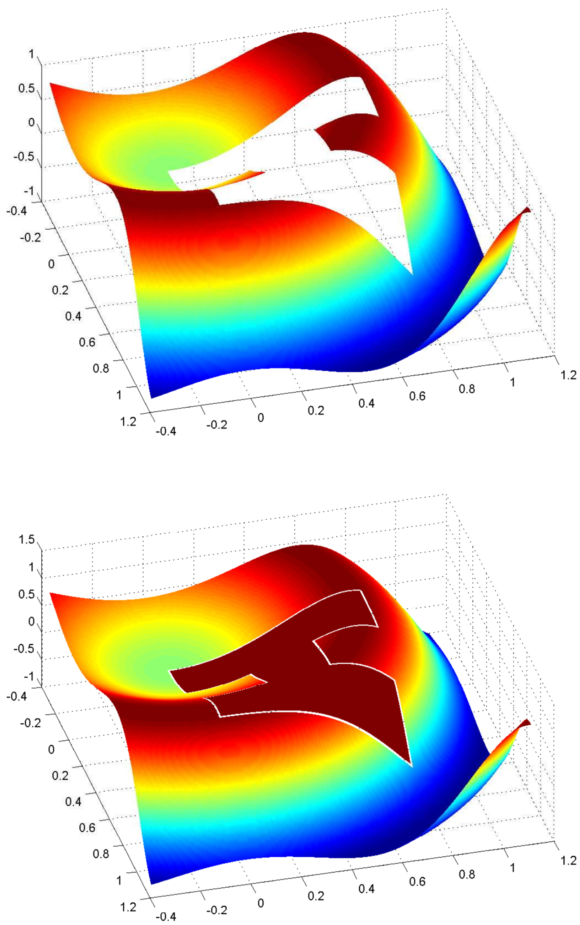

Fig. 7. Hole filling using C^1 quintic splines.

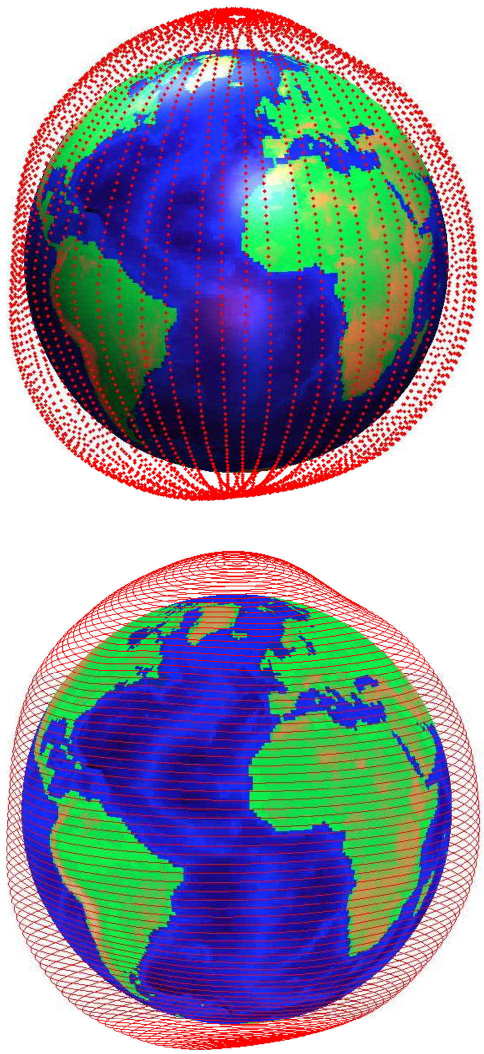

Fig. 8. Normalized simulated geopotential measurements (top) and C^1 quintic spherical spline interpolation (bottom)

3.2. Discrete Least Squares Fitting

The discrete least squares method is one of the classical methods for data fitting. Instead of polynomial fitting, we use multivariate splines. Let $\ell(f) = \sum_{i=1}^N |f(x_i,y_i)|^2$. We look for $S_f \in S_d^r(\Delta)$ such that

$$\ell(S_f - f) = \min\{\ell(s-f), s \in S_d^r(\Delta)\}.$$

S_f is called the discrete least squares fit of the given data $\{(x_i,y_i,f_i), i = 1,\cdots,N\}$ with $f_i = f(x_i,y_i)$.

To show the existence and uniqueness of the solution S_f, we need to assume

$$A_1\|s\|_{L_\infty(T)} \le \sqrt{\sum_{(x_i,y_i)\in T} |s(x_i,y_i)|^2}$$

for all $s \in S_d^r(\Delta)$ and all triangle $T \in \Delta$ (cf. [von Golitschek and Schumaker'02a]).

Theorem 5. *Suppose that the above constant A_1 is strictly positive. Then there exists a unique spline fit $S_f \in S_d^r(\Delta)$.*

Let

$$\sqrt{\sum_{(x_i,y_i)\in T} |s(x_i,y_i)|^2} \le A_2\|s\|_{L_\infty(T)}$$

for all $T \in \Delta$ and $s \in S_d^r(\Delta)$. It is easy to see that A_2 must be less than or equal to the maximal number of points per triangle. The following result was established in [von Golitschek and Schumaker'02a].

Theorem 6. *Assume that $f \in W_\infty^{m+1}(\Omega)$. Then*

$$\|S_f - f\|_{L_\infty(\Omega)} \le C\frac{A_2}{A_1}|\Delta|^{m+1}|f|_{m+1,\infty,\Omega}$$

for a constant C dependent on β, d.

Furthermore, we can show the following

Corollary of Theorem 6. Under the same assumptions above, for $|\alpha| \le m+1$,

$$\|D^\alpha(S_f - f)\|_{L_\infty(\Omega)} \le C\frac{A_2}{A_1}|\Delta|^{m+1-|\alpha|}|f|_{m+1,\infty,\Omega}$$

for a constant C dependent only on β and d.

This can be proved by using a polynomial approximation property and Markov's inequality. Details are omitted here.

Our next question is how to compute discrete least squares fits. Recall that we write each $s \in S_d^{-1}(\Delta)$ in the B-form

$$s(x,y)|_t = \sum_{i+j+k=d} c^t_{ijk} B^{d,t}_{ijk}(x,y)$$

with coefficient vector $\mathbf{c} = (c^t_{ijk}, i+j+k=d, t \in \Delta)$.

We put all smoothness conditions of $S^r_d(\Delta)$ together as

$$\mathcal{H}\mathbf{c} = 0.$$

Let $\mathcal{L}$ be an observation matrix. It is easy to see

$$\ell(s-f) = \mathbf{c}^T \mathcal{L}\mathcal{L}^T \mathbf{c} - 2\mathbf{c}^T \mathcal{L}\mathbf{f} + \mathbf{f}^T\mathbf{f}.$$

The discrete least squares spline is the solution of

$$min\{\mathbf{c}^T \mathcal{L}\mathcal{L}^T \mathbf{c} - 2\mathbf{c}^T \mathcal{L}\mathbf{f}, \text{ subject to } \mathcal{H}\mathbf{c} = 0\}.$$

By the Lagrange multipliers method, we solve

$$\begin{bmatrix} \mathcal{L}\mathcal{L}^T & \mathcal{H}^T \\ \mathcal{H} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \alpha \end{bmatrix} = \begin{bmatrix} \mathcal{L}\mathbf{f} \\ 0 \end{bmatrix}.$$

The ALW iteration introduced in the previous subsection can be applied to solve the above linear system. As before the iterative solutions converge the exact solution.

When the number of data sites is large, especially when the number of triangles is large, a computer may not be powerful enough to solve the associated linear system. We again propose a domain decomposition technique for computing an approximation of the discrete least squares spline (cf. [Lai and Schumaker'03]). That is, for $k \geq 1$, we compute $S_{f,t,k}$ such that

$$\ell_{D_k(t)}(S_{f,t,k} - f) = \min\{\ell_{D_k(t)}(s-f), s \in S^r_d(\Delta)\},$$
$$\ell_{D_k(t)}(s-f) = \sum_{(x_i,y_i)\in D_k(t)} |s(x_i,y_i) - f(x_i,y_i))^2.$$

We have the following (cf. [Lai and Schumaker'03])

Theorem 7. *Suppose that $S^r_d(\Delta)$ with $d \geq 3r+2$ over a β quasi-uniform triangulation Δ. Suppose that data values are obtained from a continuously differentiable function $f \in C^{m+1}(\Omega)$. Suppose that $A_1 > 0$ and $A_2 < \infty$ are constants such that A_2/A_1 is independent of Δ. Then there is a positive $\rho < 1$ such that*

$$\|s_f - S_{f,k}\|_{L_\infty(t)} \leq C\rho^k(k+2)|\Delta|^{m+1}|f|_{m+1,\infty,\Omega}$$

for $k \geq 1$, where C is a constant dependent only on d, β and A_2/A_1.

3.3. Penalized Least Squares Spline Method

Recall that $E(f)$ denotes a thin-plate energy functional of f and $\ell(s) = \sum_{i=1}^{N}(s(x_i, y_i) - f_i)^2$ as before. Fix $\lambda > 0$. Define $P(s) = \ell(s) + \lambda E(s)$. The PLS spline is the minimization solution $S_{f,\lambda} \in S^r_d(\Delta)$ such that

$$P(S_{f,\lambda}) = \min\{P(s), s \in S^r_d(\Delta)\}.$$

We refer to [Awanou, Lai, and Wenston'06] for a proof of the following.

Theorem 8. *Suppose that $N \geq 3$, and there exist three data sites, say $(x_i, y_i), i = 1, 2, 3$, which are not colinear. Then there exists a unique $S_{f,\lambda}$ in $S^r_d(\Delta)$ solving the above minimization problem.*

We certainly want to know if the penalized least squares fitting surface resembles the given data or not. Since $f - S_{f,\lambda} = f - S_{f,0} + S_{f,0} - S_{f,\lambda}$, we need to estimate $S_{f,0} - S_{f,\lambda}$. To do so, we introduce the following two quantities: (cf. [von Golitschek and Schumaker'02b])

$$K_1 = \sup\{\frac{E(s)^{1/2}}{\ell(s)^{1/2}}, s \in S^r_d(\Delta), s \neq 0\}$$

and

$$K_2 = \sup\{\frac{\|s\|_{L_\infty(\Omega)}}{\ell(s)^{1/2}}, s \in S^r_d(\Delta), s \neq 0\}.$$

Then in [von Golitschek and Schumaker'02b], von Golitschek and Schumaker proved the following

Theorem 9. *Let $S_{f,\lambda}$ be the Penalized Least Squares spline in $S^r_d(\Delta)$ with $d \geq 3r + 2$. Assume that K_1 and K_2 are finite. Then*

$$\|S_{f,\lambda} - S_{f,0}\|_{L_\infty(\Omega)} \leq K_2\sqrt{\lambda}E(S_{f,0}) \min\{1, K_1\sqrt{\lambda}\}.$$

We now work on estimating K_1 and K_2. It is easy to get

$$E(s) \leq \sum_{T\in\Delta} A_T\|s\|^2_{2,\infty,T} \leq \sum_{T\in\Delta} \frac{A_T}{\rho_T^4}\|s\|^2_{L_\infty(T)} \leq \frac{\beta^2}{(\rho_\Delta)^2}\frac{\ell(s)}{A_1^2}.$$

It follows that $K_1 \leq \frac{\beta}{A_1\rho_\Delta}$.

Since $\|s\|_{L_\infty(\Omega)} = \|s\|_{L_\infty(T)}$ for a triangle T,

$$\|s\|_{L_\infty(\Omega)} \leq \frac{1}{A_1}\sqrt{\sum_{(x_i,y_i)\in T}|s(x_i, y_i)|^2} \leq \frac{1}{A_1}\ell(s)^{1/2}.$$

It follows that

$$K_2 \leq \frac{1}{A_1}.$$

Theorem 10. *Let $S_{f,\lambda}$ be the PLS spline in $S^r_d(\Delta)$ with $d \geq 3r+2$. Suppose that $f \in W^{m+1}_\infty(\Omega)$ with $1 \leq m \leq d$. Then*

$$\|S_{f,\lambda} - f\|_{L_\infty(\Omega)} \leq C_1 |\Delta|^{m+1} |f|_{m+1,\infty,\Omega} + \lambda \frac{C|f|_{2,\infty,\Omega}}{A_1^2(\rho_\Delta)^2},$$

where $C_1 > 0, C_2 > 0$ are constants dependent on A_2/A_1, β and d.

To see that the convergence is linear in λ, we present some numerical experiments: For $\lambda_i = 1/2^{10+i}$, the maximum errors of S_{f,λ_i} to f are

	λ_2	λ_3	λ_4	λ_5
$S^1_5(\Delta)$	$5.466e-4$	$2.800e-4$	$1.421e-4$	$7.819e-5$
$S^1_6(\Delta)$	$5.451e-4$	$2.762e-4$	$1.408e-4$	$7.318e-5$

As we see the condition for the existence of penalized least squares spline fits is much weaker than that for the existence of the discrete least squares spline fits. However, the approximation result on penalized least squares spline fits is dependent on a very strong condition on the data sites, i.e., $A_1 > 0$. It is interesting to see if one can remove this condition while proving that the penalized least squares fits resemble the shape of the data.

Recall $\mathbf{c}$ is the coefficient vector of a spline $s \in S^{-1}_d(\Delta)$, $\mathcal{H}$ is the smoothness matrix such that $\mathcal{H}\mathbf{c} = 0$ if and only if $s \in Sr_d(\Delta)$, $\mathcal{E}$ is the energy matrix, and $\mathcal{L}$ is the observation matrix. Then the PLS spline is the minimization solution

$$min\{\mathbf{c}^T \mathcal{L}\mathcal{L}^T \mathbf{c} - 2\mathbf{c}^T \mathcal{L}\mathbf{f} + \lambda \mathbf{c}^T \mathcal{E}\mathbf{c}, \text{ subject to } \mathcal{H}\mathbf{c} = 0\}.$$

By the Lagrange multipliers method, we solve

$$\begin{bmatrix} \mathcal{L}\mathcal{L}^T + \lambda\mathcal{E} & \mathcal{H}^T \\ \mathcal{H} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c} \\ \alpha \end{bmatrix} = \begin{bmatrix} \mathcal{L}\mathbf{f} \\ 0 \end{bmatrix}.$$

We apply the ALW iteration introduced before.

When the number of triangles is large, a computer may not be powerful enough to find the PLS splines. We use a domain decomposition technique for computing an approximation of the PLS spline (cf. [Lai and Schumaker'03]). For $k \geq 1$, we compute a PLS spline $S_{f,t,k}$ such that

$$P_{D_k(t)}(S_{f,t,k}) = \min\{P_{D_k(t)}(s), s \in S^r_d(\Delta)\},$$

where

$$P_{D_k(t)}(s) = \sum_{(x_i,y_i)\in D_k(t)} |s(x_i,y_i) - f(x_i,y_i)|^2 + \lambda E(s|_{D_k(t)}).$$

Here $D_k(t) = \text{star}^k(t)$ for each triangle $t \in \triangle$. We have the following result (cf. [Lai and Schumaker'03]).

Theorem 11. *Suppose that $S^r_d(\Delta)$ with $d \geq 3r+2$ over a β quasi-uniform triangulation Δ. Suppose that data values are obtained from a continuously differentiable function $f \in C^{m+1}(\Omega)$. Suppose that $A_1 > 0$ and $A_2 < \infty$ are constants such that A_2/A_1 is independent of Δ. Then there is a positive $\rho < 1$ such that*

$$\|s_f - S_{f,k}\|_{L_\infty(t)} \leq C\rho^k((k+2)^{3/2}|\Delta|^{m+1}|f|_{m+1,\infty,\Omega} + \lambda|f|_{2,\infty,\Omega})$$

for $k \geq 1$, where C is a constant dependent only on d, β and A_2/A_1.

3.4. L_1 Spline Methods

L_1 spline methods for data fitting were proposed in [Lavery'2000]. He used C^1 cubic spline curves and bivariate C^1 cubic Sibson's elements for scattered data in 1D and grid data in 2D, respectively. Lai and Wenston in 2004 generalized the study to the scattered data in the bivariate setting. Recall that

$$\Lambda(f) = \{s \in S^r_d(\Delta), s(x_i, y_i) = f(x_i, y_i), i = 1, \cdots, N\}.$$

Let $E_1(s)$ be the L_1 energy functional, i.e.,

$$E_1(f) = \int_\Omega \left(\left| \frac{\partial^2}{\partial x^2} f \right| + 2 \left| \frac{\partial^2}{\partial x \partial y} f \right| + \left| \frac{\partial^2}{\partial y^2} f \right| \right) dxdy.$$

Find $S_f \in \Lambda(f)$ such that

$$E_1(S_f) = \min\{E_1(s), \quad s \in \Lambda(f)\}.$$

S_f is called the L_1 interpolatory spline of the given data $\{(x_i, y_i, f(x_i, y_i)), i = 1, \cdots, N\}$. A proof of the following theorem can be found in [Lai and Wenston'04]. This can be seen from the fact that the minimization functional is convex. However, the functional is not strictly convex and hence, the solution may not be unique.

Theorem 12. *Suppose that $\Lambda(f)$ is not empty. Then there exists at least one S_f solving the above minimization problem.*

The interpolatory surfaces which minimize the L_1 energy functional are indeed different from the usual L_2 minimal energy splines. Figures 9 and 10 show their differences. (These figures are borrowed from [Lai and Wenston'04].)

It is necessary to show that L_1 interpolatory splines resembles the shape of the given data. Lai in [Lai'07] proved the following

Theorem 13. *Suppose that $f \in C^2(\Omega)$. Let S_f be the L_1 interpolatory spline of the data $(x_i, y_i, f(x_i, y_i)), i = 1, \cdots, N$. Then*

$$\|S_f - f\|_{L_1(\Omega)} \leq C|\Delta|^2|f|_{2,\infty,\Omega},$$

for a constant C dependent only on β and d.

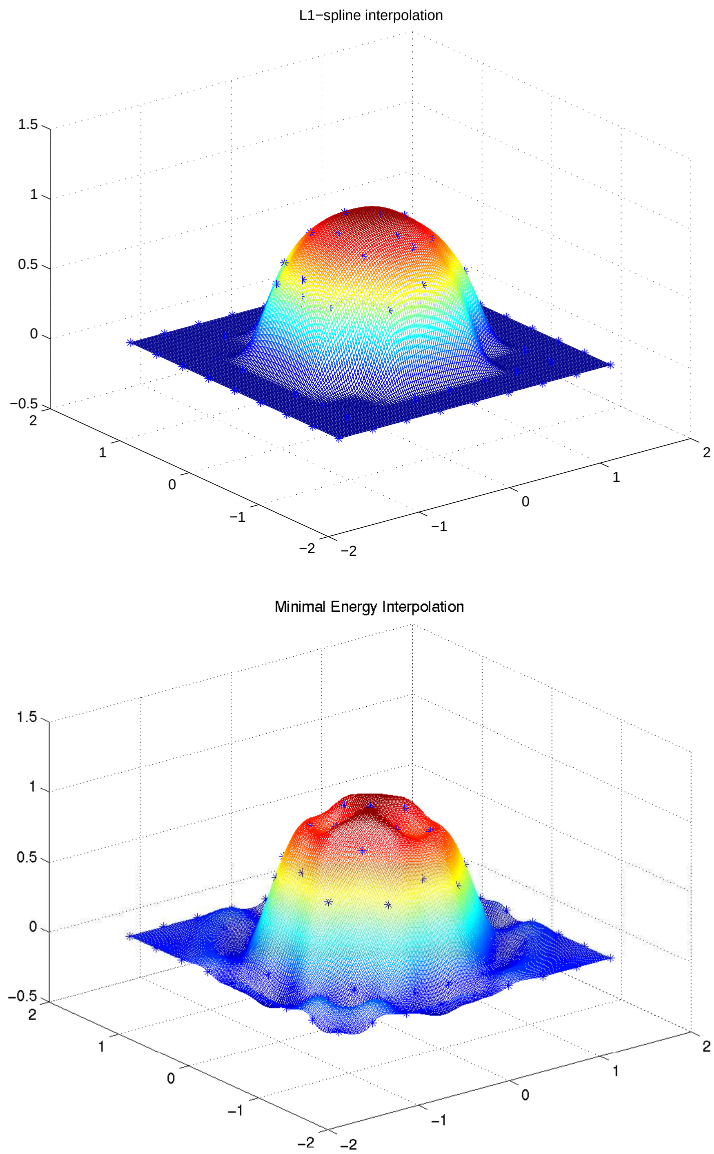

Fig. 9. L_1 interpolatory spline (the top row) and minimal energy interpolatory spline (the bottom row)

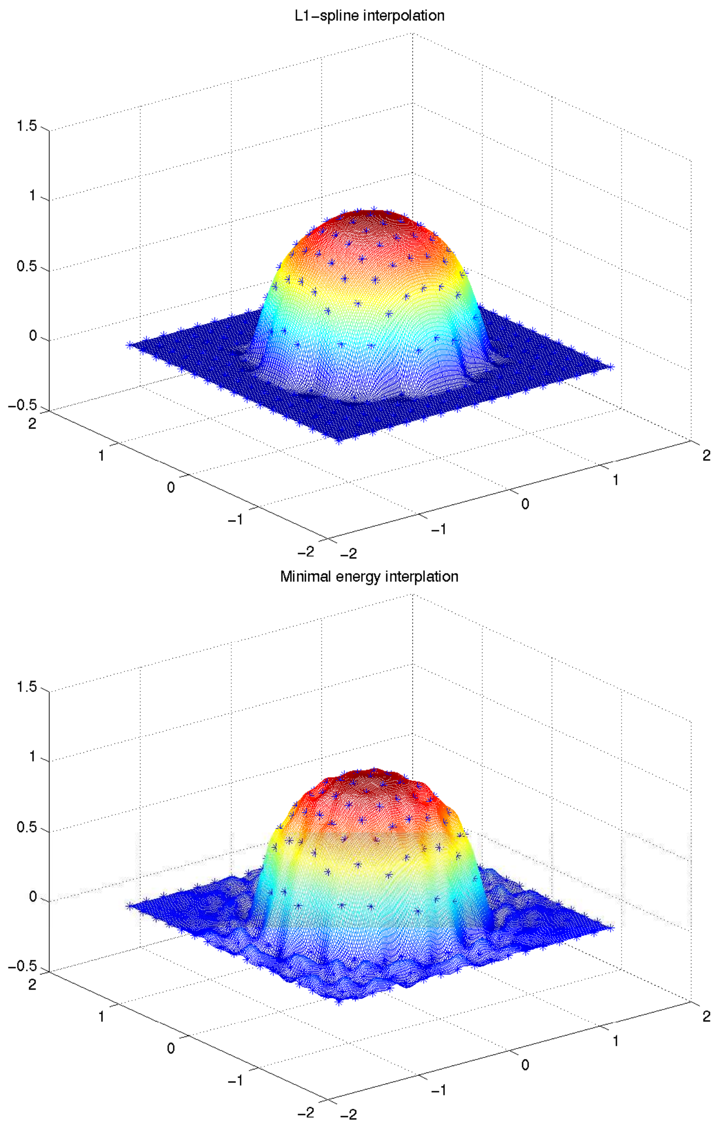

Fig. 10. L_1 interpolatory spline (the top row) and minimal energy interpolatory spline (the bottom row)

3.5. Least Absolute Deviation

For a given data set $\{(x_i, y_i, f(x_i, y_i)), i = 1, \cdots, N\}$, let

$$\ell_1(s) = \sum_{i=1}^{N} |s(x_i, y_i)|.$$

We find $S_f \in S_d^r(\Delta)$ such that

$$\ell_1(S_f - f) = \min\{\ell_1(s - f), s \in S_d^r(\Delta)\}.$$

S_f is the least absolute deviation(LAD) from the given data (cf. [Bloomfield and Steiger'83]).

Since the minimization functional is convex, there always exist a minimizer S_f (cf. [Lai and Wenston'04]). Next we would like to know how well the LAD surface resembles the given data. Let F_1 and F_2 be positive numbers such that

$$F_1 \|s\|_{L_\infty(T)} \le \sum_{(x_i, y_i) \in T} |s(x_i, y_i)| \le F_2 \|s\|_{L_\infty(T)}$$

for all $s \in S_d^r(\Delta)$ and for all $T \in \Delta$. We have the following (cf. [Lai'07]).

Theorem 14. *Suppose that two constants $F_1 > 0$ and $F_2 < \infty$ such that F_2/F_1 independent of Δ. Suppose that $f \in W_\infty^{m+1}(\Omega)$ for $0 \le m \le d$. Then*

$$\|S_f - f\|_{L_1(\Omega)} \le C|\Delta|^{m+1}|f|_{m+1,\infty,\Omega}$$

for a positive constant C dependent on F_2/F_1, β and d.

3.6. L_1 Smoothing Splines

L_1 smoothing splines are $S_f \in S_d^r(\Delta)$ which minimizes

$$\ell_1(S_f - f) + \lambda E_1(S_f) = \min\{\ell_1(s - f) + \lambda E_1(s), s \in S_d^r(\Delta)\}.$$

Since the minimization functional is convex, there exists at least one S_f solving the above minimization problem. We next need to show that S_f approximates f as the size of the triangulations goes to zero (cf. [Lai'07]).

Theorem 15. *Under the same assumptions as Theorem 14,*

$$\|S_f - f\|_{L_1(\Omega)} \le C|\Delta|^{m+1}|f|_{m+1,\infty,\Omega} + \lambda\frac{C_f}{F_1}|\Delta|^2$$

for a positive constant C dependent on F_2/F_1, β and d.

Algorithms computing these three L_1 spline methods were discussed in [Lai and Wenston'04]. The main ideas are

1) use discontinuous piecewise polynomial functions and set the smoothness conditions as side constraints;
2) convert L_1 norm minimization to a linear programming problem;
3) use Karmarkar's algorithm to solve the linear programming problem.

§4. New Research Initiatives

We now explain some new directions of research on scattered data fitting using multivariate splines.

4.1. Approximation of Convolution Functions

Suppose we know a convolution operator with known kernel $K(x,y,x',y')$,

$$f(x,y) = \int_\Omega K(x,y,x',y')g(x',y')dx'dy'.$$

Suppose that a set of data $\{(x_i, y_i, f(x_i,y_i)), i = 1, \cdots, N\}$ is given and we are required to find an approximation of g. One typical application is to compute the geopotential G near the surface of the earth from the measurement of the geopotential of a satellite at an orbital surface. We know that G is the solution of the Laplace equation:

$$G(x,y) = \int_\Omega K(x,y,x',y')g(x',y')dx'dy',$$

where K is a Poisson kernal and g is the geopotential near the earth surface. $G(x,y)$ is known at measurement locations at the orbital level taken by a satellite, CHAMP. We look for $S_g \in S^r_d(\Delta)$ minimizing

$$\min_{s\in S^r_d(\Delta)} \left(\sum_{i=1}^N (G(x_i,y_i) - \int_\Omega K(x_i,y_i,x',y')s(x',y')dx'dy' \right)^2 .$$

We say $\{(x_i,y_i), i = 1, \cdots, N\}$ are evenly distributed over Ω with respect to $S^r_d(\Delta)$: if $s \in S^r_d(\Delta)$ such that

$$\int_\Omega K(x_i,y_i,x',y')s(x',y')dx'dy' = 0,$$

for $i = 1, \cdots, N$, then $s \equiv 0$.

Theorem 16. *Suppose that the data set are evenly distributed with respect to $S^r_d(\Delta)$ for some positive integers r and $d > r$. Then there exists a unique spline $S_g \in S^r_d(\Delta)$ solving the above minimization problem.*

We say K is coercive if there exists $\alpha > 0$ such that

$$\alpha\|f\|_{L_2(\Omega)} \le \|\int_\Omega K(x,y,x',y')f(x',y')dx'dy'\|_{L_2(\Omega)}.$$

Theorem 17. *Suppose that K is bounded and coercive. Suppose that the data sites are evenly distributed. If $g \in W_\infty^{m+1}(\Omega)$ with $0 \le m \le d$, then*

$$\|S_g - g\|_{L_2(\Omega)} \le C|\Delta|^{m+1}\|g\|_{m+1,2,\Omega} + \frac{C}{N}\|g\|_{L_2(\Omega)}.$$

The above discussion can be found in [Lai'07b].

4.2. Rank Restricted Splines

Suppose $\{(x_i, y_i, f_k(x_i, y_i), i = 1, \cdots, N, k = 1, \cdots, n\}$, i.e., the targeted function f has been sampled n times over designed points $(x_i, y_i), i = 1, \cdots, N$, f has several patterns during the time period $k = 1, \cdots, n$. We look for spline functions

$$\min\{\frac{1}{n}\sum_{k=1}^{n}\left(\sum_{i=1}^{N}(f_k(x_i,y_i) - s_k(x_i,y_i))^2 + \lambda\|s_k\|_{2,2}^2\right), \quad s_k \in S_d^r(\triangle),\ \dim(\mathrm{span}(s_k, k=1,\cdots,n)) \le q\}.$$

This problem can be solved based on singular value decomposition (cf. [Guillas and Lai'07a]).

4.3. Linear Functional Approximation

In addition to the given data set

$$\{(x_i, y_i, f_k(x_i, y_i), i = 1, \cdots, N, k = 1, \cdots, n\},$$

we are also given values $v_k, k = 1, \cdots, n$. Assume that v_k is an observation of a continuous functional v at function f_k whose values $f_k(x_i, y_i)$ at designed points (x_i, y_i), $i = 1, \cdots, N$ are known. If v is linear on $L_2(\Omega)$, then there exists $\alpha \in L_2(\Omega)$ such that

$$v(f) = \langle \alpha, f\rangle, \quad \forall f \in L_2(\Omega).$$

by the Riesz representation theorem. Our aim is to approximate the linear functional v, i.e., α. One way is to find $S_{\alpha,n} \in S_d^r(\Delta)$ such that

$$S_{\alpha,n} = \arg\min_{s\in S_d^r(\Delta)} \frac{1}{n}\sum_{k=1}^{n}(v_k - \langle s, f_k\rangle)^2. \tag{1}$$

It is easy to see that the above problem is a discretization of the following problem: find $S_\alpha \in S_d^r(\triangle)$ of $v(f) = \langle \alpha, f\rangle$ such that

$$S_\alpha = \arg\min_{\beta\in S_d^r(\triangle)} E\left[(v(f) - \langle \beta, f\rangle)^2\right]. \tag{2}$$

where E is the expectation of the random variable f: $\mathcal{X} = \{f(\omega, s), \omega \in \Omega, s \in \mathcal{D}\}$, where $\mathcal{D} \subset \mathbf{R}^2$ is a bounded domain, Ω is a collection of events, and $f(\omega, \cdot) \in L_2(\mathcal{D})$ for each event ω. In [Guillas and Lai'07], we showed the following result.

Theorem 18. *Suppose that only the spline in $S_d^r(\triangle)$ which is orthogonal to the collection $\mathcal{X} \subset L_2(\mathcal{D})$ is zero. Then the minimization problem (2) has a unique solution in $S_d^r(\triangle)$.*

Furthermore we can show

Theorem 19. *Suppose that $E(\|f\|^2) \le M < \infty$ for all $f \in \mathcal{X}$, and suppose that $\alpha \in C^r(\mathcal{D})$ for $r \ge 0$. Then the solution S_α of the minimization problem (2) approximates α in the following theorem. sense:*

$$E((\langle \alpha - S_\alpha, f\rangle)^2) \le CM|\triangle|^{2r},$$

where $|\triangle|$ is the maximal length of the edges of $\triangle$.

Similarly we have the following

Theorem 20. *Suppose that only the spline function in the spline space $S_d^r(\triangle)$ perpendicular to the subspace span$\{f_1, \cdots, f_n\}$ is zero except on an event whose probability goes to zero as $n \to \infty$. Then there exists a unique $S_{\alpha,n} \in S_d^r(\triangle)$ minimizing (1).*

We now show that $S_{\alpha,n}$ approximates S_α in probability using the law of large number.

Theorem 21. *Suppose that f_ℓ, $\ell = 1, \cdots, n$ are i.i.d. and $\|f_\ell\|$ is uniformly bounded a.s. Then $S_{\alpha,n}$ converges to S_α in probability with convergence rate as in (3). That is, the probability*

$$P\left(\frac{\|S_\alpha - S_{\alpha,n}\|}{\|S_\alpha\|} \ge \epsilon\right) \le 4m^2 \exp\left(-\frac{n\gamma^2\epsilon^2}{32\kappa(A)^2 m^2 M^2}\right) + 2m \exp\left(-\frac{n\gamma^2\epsilon^2}{32\kappa(A)^2 M_b^2}\right), \tag{3}$$

where m is the dimension of spline space $S_d^r(\triangle)$, A is the coefficient matrix associated with S_α, $\kappa(A)$ denotes the condition number of matrix A, and γ is a positive constant dependent on the stability of the basis functions of $S_d^r(\triangle)$.

We refer the interested reader to [Guillas and Lai'07] for details. See [Ettinger, Guillas, and Lai'07] for further results.

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