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AN ELEMENTARY PROOF OF THE OPTIMAL RECOVERY OF THE THIN PLATE SPLINE RADIAL BASIS FUNCTION

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ABSTRACT. In many practical applications, we face the problem of reconstruction of an unknown function sampled at some data points. Among infinitely many possible reconstructions, the thin plate spline interpolation is known to be the least oscillatory one in the Beppo-Levi semi norm, when the data points are sampled in $\mathbb{R}^2$. The traditional proofs supporting the argument are quite lengthy and complicated, keeping students and researchers off its understanding. In this article, we introduce a simple and short proof for the optimal reconstruction. Our proof is unique and reguires only elementary mathematical background.

1. INTRODUCTION

Scattered data approximation has been a fast growing research area. It deals with the problem of reconstruction of an unknown function from given scattered data [1]. Naturally, it has many applications, such as surface reconstruction, fluid-structure interaction, the numerical solution of partial differential equations and parameter estimation [2]. Moreover, these applications come from such different fields as applied mathematics, computer science, biology, engineering. It is a well-established fact that a large data set is better dealt with by splines than by polynomials [3].

One of the common scattered data approximation techniques is the Radial Basis Function(RBF). A one dimensional RBF is the natural cubic spline. RBFs consist of a finite linear combination of translated basis functions. Sums of radial basis functions are typically used to approximate given functions. One advantage of RBFs is that they are independent of dimension. Since the basis functions take Euclidean distance as input, they can be extended to arbitrary dimensions. For solving practical problems of data fitting in two dimensions, one of the most popular radial basis functions is the thin plate spline(TPS). The optimality and solvability of radial basis function interpolation is already proved in general case, however the proof is quite complex [4, 5]. In this paper, we introduce a proof of the optimality in the sense of the L^2-minimum norm and solvability of the interpolation with TPS, just with an elementary mathematical background.

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In a traditional textbook of RBF by Wendland [5, 6], the understanding of the optimal recovery of TPS can be obtained through seven theorems that takes up about ten pages. The proof requires the concept of completely monotone, Helly's theorem, Hausdorff-Bernstein-Widder theorem, Schoenberg theorem and the Micchelli's theorem that may sound new to most students and researchers.

We can also find another proof in the paper by Madych and Nelson which generalizes the approach of Bochner's [7, 8] to the case of conditionally positive definite functions. It consists of eight theorems that take up about eight pages [9]. The precise characterization of Madych-Nelson requires the concepts of generalized fourier transforms. Compare to the Schoenberg-Micchelli approach, the proof of the basic result of Madych-Nelson is rather easy but it is technically difficult to apply the general result to specific basis functions [9, 10, 11]. Bochner's characterization provides direct proofs for RBFs but is not applicable to conditionally positive definite functions [12, 13].

Contrary to the aforementioned references, this article introduces a simple and short proof that requires only elmentary mathematical background. In section 2, we briefly review the formulation of the optimal recovery problem and the definition of the TPS interpolation. In section 3, we prove that the interpolation solves the optimal recovery problem.

2. Problem setting

Given function values $\{f_1, ..., f_N\}$ on a discrete set $\{\mathbf{x}_1, ..., \mathbf{x}_N\}$ of scattered locations $\mathbf{x}_j \in \mathbb{R}^2$, we want to reconstruct a function f in defined in $\mathbb{R}^2$. Among infinitely many smooth functions that pass through all the data, we seek the least oscillatory one. The oscillation is measured by the magnitude of the second order derivatives in L^2-norm. The measurement of the oscillation is through the Beppo-Levi semi-norm [14], which is denoted by $||\cdot||_V$ throughout this paper. The space V is an inner product space defined as below.

$$V:=\{g:\mathbb{R}^2\to\mathbb{R}|g\in C(\mathbb{R}^2),\ g_{xx},g_{xy},g_{yy}\in L^2(\mathbb{R}^2)\}$$

$$<g_1,g_2>_V:=\int_{\mathbb{R}^2}\frac{\partial^2 g_1}{\partial x^2}\frac{\partial^2 g_2}{\partial x^2}+2\frac{\partial^2 g_1}{\partial x\partial y}\frac{\partial^2 g_2}{\partial x\partial y}+\frac{\partial^2 g_1}{\partial y^2}\frac{\partial^2 g_2}{\partial y^2}d\mathbf{x}$$

$$\parallel g\parallel_V:=\sqrt{<g,g>_V}$$

The problem of reconstruction can be cast into the following optimization problem for finding $g^\star$ in M.

$$M:=\{g\in V|g(\mathbf{x}_i)=f(\mathbf{x}_i)\quad\forall i\},\ \ g^\star=\underset{g\in M}{argmin}\parallel g\parallel_V^2 \tag{2.1}$$

The solution of the above optimization problem is known as the TPS interpolation. The interpolation is called radial basis function interpolation, because it is a sum of translated basis functions that are radially symmetric. In specific, for the data points, the TPS interpolation takes the following form.

$$g^{TPS}(\mathbf{x}) = \sum_{j=1}^{N} \alpha_j \phi(\parallel \mathbf{x} - \mathbf{x}_j \parallel) + \beta_1 x + \beta_2 y + \beta_0, \tag{2.2}$$

where $\phi(r) = r^2$ log(r). The coefficients are uniquely determined by the following conditions.

$$\begin{aligned} &g^{TPS}(\mathbf{x}_i) = f(\mathbf{x}_i) \text{ for } i = 1, 2, ..., N \\ &\sum_{j=1}^{N} \alpha_j = 0, \ \sum_{j=1}^{N} \alpha_j \mathbf{x}_j = \mathbf{0} \end{aligned} \tag{2.3}$$

As described in the introduction, it has been a painstaking and hard learning process to understand why the TPS interpolation is the solution of the optimization problem, i.e., $g^\star = g^{TPS}$. In the next section, we introduce a simple and short proof that requires only elementary mathematical background.

3. Elementary proof

We provide an elementary proof that shows why the TPS interpolation (2.2) is the solution of the optimization problem (2.1), i.e., $g^\star = g^{TPS}$. We begin with a standard lemma for the distance minimization in an inner-product space.

Lemma 1. $g^\star = \underset{g \in M}{argmin} \parallel g \parallel_V^2$ *if and only if* $< g^\star, v >_V = 0, \forall v \in M_0$. *Here* $M_0 := \{g \in V | g(\mathbf{x}_i) = 0 \quad \forall i\}$.

Proof. $(\Rightarrow)$ $0 \neq \forall v \in M_0, \ \forall \epsilon \in \mathbb{R}, \ g^\star + \epsilon v \in M$. By the assumption that $g^\star$ is the minimizer,

$$\begin{aligned} \parallel g^\star + \epsilon v \parallel_V^2 \ &\geq \parallel g^\star \parallel_V^2, \ \forall \epsilon \in \mathbb{R}, \\ \parallel v \parallel_V^2 \epsilon^2 + 2 < g^\star, v >_V \epsilon \ &\geq \ 0, \ \forall \epsilon \in \mathbb{R}. \end{aligned}$$

The quadratic equation does not have a real root, and its discriminant should be nonpositive, $< g^\star, v >_V^2 \leq 0$. Since $< g^\star, v >_V^2 \ \geq \ 0$, finally we get $< g^\star, v >_V \ = 0$.

$(\Leftarrow)$ $\forall g \in M, \ g - g^\star \in M_0$. Using the orthogonality assumption,

$$\begin{aligned} \parallel g \parallel_V^2 &= \parallel g^\star + (g - g^\star) \parallel_V^2 \\ &= \parallel g^\star \parallel_V^2 + \parallel g - g^\star \parallel_V^2 \geq ||g^\star||_V^2. \end{aligned}$$

□

Before we provide the main theorem, we list the following calculation of elementary differentiations.

- $\nabla \phi(\parallel \mathbf{x} - \mathbf{x}_i \parallel) = (2\log(\parallel \mathbf{x} - \mathbf{x}_i \parallel) + 1)(\mathbf{x} - \mathbf{x}_i)$
- $\nabla(\Delta \phi(\parallel \mathbf{x} - \mathbf{x}_i \parallel)) = 4 \frac{\mathbf{x} - \mathbf{x}_i}{\|\mathbf{x} - \mathbf{x}_i\|^2}$

- $\Delta\phi(\| \mathbf{x}-\mathbf{x}_i \|)$ =4log$(\| \mathbf{x}-\mathbf{x}_i \|)+4$
- $\nabla^2\phi(\| \mathbf{x}-\mathbf{x}_i \|)$=(2log$(\| \mathbf{x}-\mathbf{x}_i \|)+1)I+\frac{2(\mathbf{x}-\mathbf{x}_i)(\mathbf{x}-\mathbf{x}_i)^T}{\|\mathbf{x}-\mathbf{x}_i\|^2}$
- $\Delta^2\phi(\| \mathbf{x}-\mathbf{x}_i \|)=0$

Theorem 3.1. *The TPS interpolation in equation* (2.2) *is the optimal solution of the problem* (2.1).

Proof. We prove the argument in two steps. In the first step, we show $g^{TPS}\in M$. In the second, we show the orthogonality $g^{TPS}\perp M_0$, which implies by the lemma on the optimality, $g^{TPS}=\underset{g\in M}{argmin}\ \| g \|_V^2$.

(Step 1) : Show that $g^{TPS}\in M$.

Since $g^{TPS}(\mathbf{x}_i)=f_i$ by equation (2.1), it is enough to check the L^2-integrability only. We want to show those elements are in L^2, $g_{xx}^{TPS},\ g_{xy}^{TPS},\ g_{yy}^{TPS}\in L^2(\mathbb{R}^2)$, constituting the Hessian matrix $\nabla^2 g^{TPS}$.

$$\nabla^2 g^{TPS}(\mathbf{x})=\underbrace{\sum_{i=1}^N \alpha_i(2\log(\| \mathbf{x}-\mathbf{x}_i \|)+1)I}_{\text{(a)}}+\underbrace{2\sum_{i=1}^N \alpha_i\frac{(\mathbf{x}-\mathbf{x}_i)(\mathbf{x}-\mathbf{x}_i)^T}{\| \mathbf{x}-\mathbf{x}_i \|^2}}_{\text{(b)}}$$

Since $L^2(\mathbb{R}^2)$ is a vector space, we may show that all the elements of $\nabla^2 g^{TPS}$ are L^2-integrable by separately checking that the two components (a) and (b) are so.

(Step 1-a) : The component (a) is a scalar times constant matrix, hence it is enough to check the L^2-integrability of the scalar component. Using the condition $\sum_{i=1}^N \alpha_i=0$ in equation (2.3), the scalar is simplified as $\sum_{i=1}^N 2\alpha_i\log(\| \mathbf{x}-\mathbf{x}_i \|)$. We can simply check the integrability of $log(\| \mathbf{x}-\mathbf{x}_i \|)$ around the singularity $\mathbf{x_i}$ as

$$\int\limits_{\|\mathbf{x}-\mathbf{x}_i\|<1} \log\left(\|\mathbf{x}-\mathbf{x}_i\|\right)^2 d\mathbf{x}=2\pi\int\limits_0^1 (\log r)^2\, r\, dr=\frac{\pi}{2}.$$

Let $M=\max_i \| \mathbf{x}_i \|$, then $\sum_{i=1}^N \alpha_i\log\left(\|\mathbf{x}-\mathbf{x}_i\|\right)$ is L^2-integrable, since the disk is compact and it is integrable around all the singularity points.

For given $\mathbf{x}$ and $\mathbf{x}_i$, consider one-dimensional function $f(t)=\log\left(\|\mathbf{x}-t\mathbf{x}_i\|\right)$. Applying the Taylor remainder theorem to the function at $t=0$ gives $f(1)=f(0)+f'(0)+\frac{1}{2}f''(\xi_i)$, which is

$$\log\left(\|\mathbf{x}-\mathbf{x}_i\|\right)=\log\left(\|\mathbf{x}\|\right)-\frac{\mathbf{x}\cdot\mathbf{x}_i}{\|\mathbf{x}\|^2}+\frac{1}{2}\frac{\|\mathbf{x}_i\|^2}{\|\mathbf{x}-\xi_i\mathbf{x}_i\|^2}-\frac{\left((\mathbf{x}-\xi_i\mathbf{x}_i)\cdot\mathbf{x}_i\right)^2}{\|\mathbf{x}-\xi_i\mathbf{x}_i\|^4},$$

for some $\xi_i\in(0,1)$. Using the conditions $\sum_i\alpha_i=0$ and $\sum_i\alpha_i\mathbf{x}_i=\mathbf{0}$, we get

$$\sum_{i=1}^N \alpha_i\log\left(\|\mathbf{x}-\mathbf{x}_i\|\right)=\sum_{i=1}^N \alpha_i\left[\frac{1}{2}\frac{\|\mathbf{x}_i\|^2}{\|\mathbf{x}-\xi_i\mathbf{x}_i\|^2}-\frac{\left((\mathbf{x}-\xi_i\mathbf{x}_i)\cdot\mathbf{x}_i\right)^2}{\|\mathbf{x}-\xi_i\mathbf{x}_i\|^4}\right].$$

Outside the disc, $\|\mathbf{x}\| > 2M$ and

$$\frac{1}{2}\|\mathbf{x}\| \le \|\mathbf{x}\| - M \le \|\mathbf{x} - \xi_i \mathbf{x}_i\| \le \|\mathbf{x}\| + M \le 2\|\mathbf{x}\|.$$

The integrand is bounded by an L^2-integrable function outside the disc as below, which completes the proof of step 1-a.

$$\left|\frac{1}{2}\frac{\|\mathbf{x}_i\|^2}{\|\mathbf{x} - \xi_i \mathbf{x}_i\|^2} - \frac{((\mathbf{x} - \xi_i \mathbf{x}_i)\cdot \mathbf{x}_i)^2}{\|\mathbf{x} - \xi_i \mathbf{x}_i\|^4}\right| \le \frac{2M^2}{\|\mathbf{x}\|^2} + \frac{64M^2}{\|\mathbf{x}\|^2}$$

(Step 1-b) : The integrand of component (b) is matrix-valued. All the elements of the matrix $(\mathbf{x} - \mathbf{x}_i)(\mathbf{x} - \mathbf{x}_i)^T / \|\mathbf{x} - \mathbf{x}_i\|^2$ are bounded by one. Hence, it is integrable on the disc $\{\mathbf{x} | \|\mathbf{x}\| < 2M\}$, although the integrand is singular at each $\mathbf{x}_i$. Outside the disc, similar to step 1-a, we take the following matrix-valued function.

$$g(t) = \frac{(\mathbf{x} - t\mathbf{x}_i)(\mathbf{x} - t\mathbf{x}_i)^T}{\|\mathbf{x} - t\mathbf{x}_i\|^2}$$

By the Taylor remainder theorem, we have $g(1) = g(0) + g'(0) + \frac{1}{2}g''(\xi_i)$ for some $\xi_i \in (0,1)$, which leads as

$$\begin{aligned}
\frac{(\mathbf{x} - \mathbf{x}_i)(\mathbf{x} - \mathbf{x}_i)^T}{\|\mathbf{x} - \mathbf{x}_i\|^2} \quad = \quad & \frac{\mathbf{x}\mathbf{x}^T}{\|\mathbf{x}\|^2} - \frac{\mathbf{x}_i\mathbf{x}^T + \mathbf{x}_i\mathbf{x}^T}{\|\mathbf{x}\|^2} + \frac{2\mathbf{x}\cdot\mathbf{x}_i}{\|\mathbf{x}\|^4}\mathbf{x}\mathbf{x}^T + \frac{\mathbf{x}_i\mathbf{x}_i^T}{\|\mathbf{x} - \xi_i\mathbf{x}_i\|^2} \\
& -2\frac{\mathbf{x}_i(\mathbf{x} - \xi_i\mathbf{x}_i)^T + (\mathbf{x} - \xi_i\mathbf{x}_i)\mathbf{x}_i^T}{\|\mathbf{x} - \xi_i\mathbf{x}_i\|^4}(\mathbf{x} - \xi_i\mathbf{x}_i)\cdot\mathbf{x}_i \\
& -\frac{\|\mathbf{x}_i\|^2(\mathbf{x} - \xi_i\mathbf{x}_i)(\mathbf{x} - \xi_i\mathbf{x}_i)^T}{\|\mathbf{x} - \xi_i\mathbf{x}_i\|^4} \\
& +4\frac{((\mathbf{x} - \xi_i\mathbf{x}_i)\cdot\mathbf{x}_i)^2(\mathbf{x} - \xi_i\mathbf{x}_i)(\mathbf{x} - \xi_i\mathbf{x}_i)^T}{\|\mathbf{x} - \xi_i\mathbf{x}_i\|^6}.
\end{aligned}$$

Using the conditions $\sum_{i=1}^N \alpha_i = 0$ and $\sum_{i=1}^N \alpha_i\mathbf{x}_i = \mathbf{0}$, we have

$$\sum_{i=1}^N \alpha_i\left(\frac{\mathbf{x}\mathbf{x}^T}{\|\mathbf{x}\|^2} - \frac{\mathbf{x}_i\mathbf{x}^T + \mathbf{x}_i\mathbf{x}^T}{\|\mathbf{x}\|^2} + \frac{2\mathbf{x}\cdot\mathbf{x}_i}{\|\mathbf{x}\|^4}\mathbf{x}\mathbf{x}^T\right) = \mathbf{0}.$$

For a matrix A, let us denote the elementwise maximum by $\|A\|_\infty = \max_{i,j}|A_{ij}|$. For a rank-one matrix $\mathbf{x}\mathbf{y}^T$, we get $\left\|\mathbf{x}\mathbf{y}^T\right\|_\infty \le \|\mathbf{x}\|\|\mathbf{y}\|$. Outside the disk, $\frac{1}{2}\|\mathbf{x}\| \le \|\mathbf{x} - \xi_i\mathbf{x}_i\| \le$

$2\left\|\mathbf{x}\right\|$ and each integrand is bounded by an L^2 integrable function as below.

$$\begin{aligned}
\left\|\frac{\mathbf{x}_i\mathbf{x}_i^T}{\left\|\mathbf{x}-\xi_i\mathbf{x}_i\right\|^2}\right\|_\infty &\leq \frac{4M^2}{\left\|\mathbf{x}\right\|^2} \\
\left\|\frac{\mathbf{x}_i\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)^T+\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)\mathbf{x}_i^T}{\left\|\mathbf{x}-\xi_i\mathbf{x}_i\right\|^4}\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)\cdot\mathbf{x}_i\right\|_\infty &\leq \frac{128M^2}{\left\|\mathbf{x}\right\|^2} \\
\left\|\frac{\left\|\mathbf{x}_i\right\|^2\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)^T}{\left\|\mathbf{x}-\xi_i\mathbf{x}_i\right\|^4}\right\|_\infty &\leq \frac{64M^2}{\left\|\mathbf{x}\right\|^2} \\
\left\|\frac{\left(\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)\cdot\mathbf{x}_i\right)^2\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)\left(\mathbf{x}-\xi_i\mathbf{x}_i\right)^T}{\left\|\mathbf{x}-\xi_i\mathbf{x}_i\right\|^6}\right\|_\infty &\leq \frac{256M^2}{\left\|\mathbf{x}\right\|^2}
\end{aligned}$$

Therefore, step 1-b is complete and so is step 1.

(Step 2) : We show that $g^{TPS} \perp M_0$.

In step-1, it was shown that each element of $\nabla^2 g^{TPS}$ is L^2 integrable. For any $v \in M_0$, the integral of $\left\langle g^{TPS}, v\right\rangle_V = \int_{\mathbb{R}^2} \nabla^2 g^{TPS} : \nabla^2 v \, d\mathbf{x}$ is thus finite, and the following integration-by-parts are valid.

$$\begin{aligned}
\left\langle g^{TPS}, v\right\rangle_V &= \sum_{i=1}^N \alpha_i \int_{\mathbb{R}^2} \nabla^2\phi\left(\left\|\mathbf{x}-\mathbf{x}_i\right\|\right) : \nabla^2 v \, d\mathbf{x} \\
&= \lim_{\epsilon\to 0^+} \sum_{i=1}^N \alpha_i \int_{\left\|\mathbf{x}-\mathbf{x}_i\right\|>\epsilon} \nabla^2\phi\left(\left\|\mathbf{x}-\mathbf{x}_i\right\|\right) : \nabla^2 v \, d\mathbf{x} \\
&= \lim_{\epsilon\to 0^+} \sum_{i=1}^N \alpha_i \left(\int_{\left\|\mathbf{x}-\mathbf{x}_i\right\|>\epsilon} -\nabla\left(\Delta\phi\right)\cdot\nabla v \, d\mathbf{x} + \int_{\left\|\mathbf{x}-\mathbf{x}_i\right\|=\epsilon} \mathbf{n}^T\nabla^2\phi\cdot\nabla v \, d\mathbf{x} \right) \\
&= \lim_{\epsilon\to 0^+} \sum_{i=1}^N \alpha_i \left(\int_{\left\|\mathbf{x}-\mathbf{x}_i\right\|=\epsilon} -v\nabla\left(\Delta\phi\right)\cdot\mathbf{n} \, ds + \int_{\left\|\mathbf{x}-\mathbf{x}_i\right\|=\epsilon} \nabla v\cdot\left(\nabla^2\phi\right)\cdot\mathbf{n} \, ds \right)
\end{aligned}$$

Note that $\Delta^2\phi = 0$ was used in the above. On $\|\mathbf{x} - \mathbf{x}_i\| = \epsilon$, $\nabla(\Delta\phi) = -\frac{4}{\epsilon}\mathbf{n}$ and $\nabla^2\phi = (2\log\epsilon + 1)\, I + 2\mathbf{n}\mathbf{n}^T$, which give

$$
\begin{aligned}
\left\langle g^{TPS}, v\right\rangle_V &= \lim_{\epsilon\to 0^+}\sum_{i=1}^{N}\alpha_i\left(\frac{4}{\epsilon}\int\limits_{\|\mathbf{x}-\mathbf{x}_i\|=\epsilon} v\, ds + (2\log\epsilon + 3)\int\limits_{\|\mathbf{x}-\mathbf{x}_i\|=\epsilon}\nabla v\cdot\mathbf{n}\, ds\right)\\
&= 8\pi\sum_{i=1}^{N}\alpha_i v(\mathbf{x}_i) + \lim_{\epsilon\to 0^+}(2\log\epsilon + 3)\left(\sum_{i=1}^{N}\alpha_i\int\limits_{\|\mathbf{x}-\mathbf{x}_i\|<\epsilon}\Delta v\, d\mathbf{x}\right)\\
&= 0.
\end{aligned}
$$

In the above, we used $v(\mathbf{x}_i) = 0, \forall i$ and $\left|\int_{\|\mathbf{x}-\mathbf{x}_i\|<\epsilon}\Delta v\, d\mathbf{x}\right| \leq \pi\epsilon^2\max|\Delta v|$.
$\therefore$ By step 1 and step 2, $g^{TPS} \equiv g^\star$ is the optimal form of the solution. □

4. CONCLUSION

We introduced a simple and short proof for the optimal reconstruction of the TPS interpolation. Our proof is unique and requires only elementary mathematical background such as integraion-by-parts and Taylor's remainder theorem. Contrary to the great importance of the optimal reconstruction, the traditional proofs are quite complex and require very exotic theorems. Our simple and elementary proof will help many students and researchers to easily understand the optimal property of the TPS interpolation and make successes in its applications.

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