On the Bijectivity of Thin-plate Splines.

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Abstract

The thin-plate spline (TPS) has been widely used in a number of areas such as image warping, shape analysis and scattered data interpolation. Introduced by Bookstein [1], it is a natural interpolating function in two dimensions, parameterized by a finite number of landmarks. However, even though the thin-plate spline has a very elegant intuitive interpretation as well as mathematical formulation it has no inherent restriction to prevent folding, i.e. a non-bijective interpolating function. In this paper we discuss some of the properties of the set of parameterizations that form bijective thin-plate splines, such as convexity and boundness. Methods for finding sufficient as well as necessary conditions for bijectivity are also presented.

1 Introduction

The thin-plate spline (TPS) is a natural choice of interpolating function in two dimensions and has been a commonly used tool in computer vision for over a decade. Its attraction might include a the elegant mathematical formulation along with a very natural interpretation, as thin-plate splines can be viewed as modeling the bending of a thin metal plate under point constraints. However there are disadvantages, firstly it might be a very computationally expensive tool. Secondly, a TPS-mapping has no inherent restriction to prevent folding from occurring, i.e. there are no constraints on when the mapping is non-bijective. Since, in the context of computer vision, non-bijective deformations of images are quite uncommon in natural images (see figs. 1,2), it is the latter issue that will be addressed in this paper.

Figure 1: Bijective mapping.

The motivation for this work is that we wanted to perform registration between images using thin-plate splines. That is, the optimization problem of finding a bijective deformation that minimizes some similarity function between image pairs. Therefore, to obtain the optimization constraints we need to learn more about this set of bijective thin-plate spline deformations. Furthermore, as are working within an optimization framework we are also interested in other properties of the set defined by the bijectivity constraints, such as if this set is convex, bounded and/or star-shaped.

2 The Thin-Plate Spline and bijectivity constraints.

The thin-plate spline mapping $g : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ given by a set of k control points (or landmarks) T and a set of k destination points Y such that $g(T) = Y$ is, with the metal plate analogy in mind, the transformation that minimizes the roughness penalty (or bending energy)

$$\int_{\mathbb{R}^2} \left(\frac{\partial^2 g}{\partial \mathbf{x}^2} \right) d\mathbf{x} \quad (1)$$

It has been shown by Kent and Mardia [2] that

Figure 2: Non-bijective mapping.

a bivariate function ϕ in the form (for details see [1])

$$\begin{aligned} \phi_{\mathbf{T}, \mathbf{Y}}(\mathbf{x}) &= (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}))^T = c + A\mathbf{x} + \\ &+ W(\sigma(\mathbf{x} - T_1), \dots, \sigma(\mathbf{x} - T_k)) = \\ &= \begin{bmatrix} W^T & c & A \end{bmatrix} \begin{bmatrix} s(\mathbf{x}) \\ 1 \\ \mathbf{x} \end{bmatrix} \end{aligned} \quad (2)$$

with

$$s(h) = ||h||^2 \log(||h||), \quad (3)$$

$$\begin{bmatrix} W^T & c & A \end{bmatrix} = [\mathbf{Y}^T \ \mathbf{0} \ \mathbf{0}] \Gamma_{\mathbf{T}}^{-1} \quad (4)$$

minimizes eq. (1)

Combining this, the transformation can be written as

$$\phi_{\mathbf{T}, \mathbf{Y}}(\mathbf{x}) = [\mathbf{Y}^T \ \mathbf{0} \ \mathbf{0}] \Gamma_{\mathbf{T}}^{-1} \begin{bmatrix} s(\mathbf{x}) \\ 1 \\ \mathbf{x} \end{bmatrix} = \mathbf{Y}^T N_{\mathbf{T}}(\mathbf{x}) \quad (5)$$

This gives us a deformation ϕ that for a fixed set of control points $\mathbf{T}$ is parameterized (linearly) by the destination points $\mathbf{Y}$. And we are interested in knowing for which $\mathbf{Y}$ do we get a bijective deformation, i.e the set

$$\Omega_{\mathbf{T}} = \{ \mathbf{Y} \in \mathbb{R}^{2k} | \phi_{\mathbf{T}, \mathbf{Y}}(\mathbf{x}) \text{ is bijective} \}$$

Such a mapping $\phi : \mathbb{R} \rightarrow \mathbb{R}$ is bijective if and only if its functional determinant $|J(\phi)|$ is non-zero. Using (5) we get

$$|J(\phi)| = \begin{vmatrix} \frac{\partial \phi_1}{\partial x_1} & \frac{\partial \phi_1}{\partial x_2} \\ \frac{\partial \phi_2}{\partial x_1} & \frac{\partial \phi_2}{\partial x_2} \end{vmatrix} = \dots = \hat{\mathbf{Y}}^T B_{\mathbf{T}}(\mathbf{x}) \hat{\mathbf{Y}} \quad (6)$$

with

$$B_{\mathbf{T}}(\mathbf{x}) = \begin{bmatrix} 0 & D(\mathbf{x}) \\ -D(\mathbf{x}) & 0 \end{bmatrix} \quad (7)$$

$$\begin{cases} D(\mathbf{x}) &= b_{x_1}(\mathbf{x})b_{x_2}(\mathbf{x})^T - b_{x_2}(\mathbf{x})b_{x_1}(\mathbf{x})^T \\ b_{x_1}(\mathbf{x}) &= \Gamma_{11} \frac{\partial s}{\partial x_1}(\mathbf{x}) + \Gamma_1 \\ b_{x_2}(\mathbf{x}) &= \Gamma_{11} \frac{\partial s}{\partial x_2}(\mathbf{x}) + \Gamma_2 \end{cases} \quad (8)$$

Where $\hat{\mathbf{Y}}$ is the vectorized version of the k -by-2 matrix $\mathbf{Y}$. $B_{\mathbf{T}}(\mathbf{x})$ is a $2k$ -by- $2k$ symmetric, indefinite, rank-four matrix with zeros in the diagonal and non-zero eigenvalues $\lambda_{\mathbf{T}}(\mathbf{x})$, $\lambda_{\mathbf{T}}(\mathbf{x})$, $-\lambda_{\mathbf{T}}(\mathbf{x})$, $-\lambda_{\mathbf{T}}(\mathbf{x})$. So for each point $\mathbf{x} \in \mathbb{R}^2$ we get a quadratic constraint on $\mathbf{Y}$, ($\hat{\mathbf{Y}}^T B_{\mathbf{T}}(\mathbf{x}) \hat{\mathbf{Y}} \neq 0$) for local bijectivity. For ϕ to be globally bijective this constraint must either be > 0 , $\forall \mathbf{x} \in \mathbb{R}^2$ or < 0 , $\forall \mathbf{x} \in \mathbb{R}^2$. $\Omega_{\mathbf{T}}$ can thus be written

$$\Omega_{\mathbf{T}} = \{ \mathbf{Y} \in \mathbb{R}^{2k} | \hat{\mathbf{Y}}^T B_{\mathbf{T}}(\mathbf{x}) \hat{\mathbf{Y}} > 0, \forall \mathbf{x} \in \mathbb{R}^2 \text{ or } \hat{\mathbf{Y}}^T B_{\mathbf{T}}(\mathbf{x}) \hat{\mathbf{Y}} < 0, \forall \mathbf{x} \in \mathbb{R}^2 \}$$

Seeing that if $\mathbf{Y} \in \Omega_{\mathbf{T}}$ then $-\mathbf{Y} \in \Omega_{\mathbf{T}}$, it does, without loss of generality, suffice to examine

$$\Omega_{\mathbf{T}}^+ = \{ \mathbf{Y} \in \mathbb{R}^{2k} | \hat{\mathbf{Y}}^T B_{\mathbf{T}}(\mathbf{x}) \hat{\mathbf{Y}} > 0, \forall \mathbf{x} \in \mathbb{R}^2 \}$$

(with $\Omega_{\mathbf{T}}^-$ defined similarly, we can write $\Omega_{\mathbf{T}} = \Omega_{\mathbf{T}}^+ \cup \Omega_{\mathbf{T}}^-$.)

Figure 3: The resulting quadratic constraints on a subset of $\mathbf{Y}$ imposed by three points in $\mathbb{R}^2$. ($\mathbf{x}$): The control points, (*): The three arbitrarily chosen points in $\mathbb{R}^2$.

So the sought after set is the intersection of an infinite number of indefinite (and non-convex) quadratic forms each given by eq.(6).

3 Convexity of $\Omega_{\mathbf{T}}^+$ and other Properties.

As previously mentioned, we wish to use these bijectivity constraints within an optimization context and that therefore the convexity of $\Omega_{\mathbf{T}}^+$ is of great interest. In general, one would not expect that the intersection of non-convex sets would result in a convex set. Empirical observations made seem to agree with this suspicion. For certain simple control configurations $\mathbf{T}$, non-convexity of $\Omega_{\mathbf{T}}^+$ can quite easily be shown. A natural continuation is to ask if imposing some further restrictions on $\mathbf{Y}$ can result in $\Omega_{\mathbf{T}}^+$ becoming convex? For instance, if one allows all but three (linearly independent)

points in $\mathbf{Y}$ freedom, (one can view this as eliminating affine transformations of $\mathbf{Y}$ from $\Omega_{\mathbf{T}}^+$). Once again experiments have indicated that our set still is non-convex. Other similar constraints on the destination points, such as “locking” points close to the border of the convex hull of $\mathbf{Y}$, have also resulted in a non-convex set. However, instances when convexity occur do exist. If only one control point is let loose, then $\Omega_{\mathbf{T}}^+$, owing to the special form of $B_{\mathbf{T}}(\mathbf{x})$ in eq.(6), becomes a polytope, see fig. 4.

Figure 4: The resulting bijectivity constraints when only allowing one destination point to move.

Even though many of these observations remain to be proven they do provide strong indications that $\Omega_{\mathbf{T}}^+$ in general is a non-convex set.

Regarding the boundness of $\Omega_{\mathbf{T}}^+$. It is known that for affine transformations $a(\mathbf{Y})$ the following holds

$$\phi_{\mathbf{T},a(\mathbf{Y})}(\mathbf{x}) = a(\phi_{\mathbf{T},\mathbf{Y}}(\mathbf{x})) \quad (9)$$

So if $\mathbf{Y} \in \Omega_{\mathbf{T}}^+$ and $a(\mathbf{Y})$ nonsingular then $a(\mathbf{Y}) \in \Omega_{\mathbf{T}}^+$. Hence $\Omega_{\mathbf{T}}^+$ is clearly unbounded. We are however convinced that it can be proven that under an affine elimination, as previously described, the set becomes bounded.

Experiments have also indicated that $\Omega_{\mathbf{T}}^+$ might be star-shaped, that is that the intersection between any line passing through $\mathbf{T}$ and $\Omega_{\mathbf{T}}^+$ is a convex set. Further study of this property is still required though.

Although the properties discussed in this section have mainly been observed through experimentation on a very limited number of different control- and destination configurations it does provide us with the opportunity to get a better understanding of what kind of object we are working with. Which, in summation, is a high-dimensional, non-convex, unbounded monstrosity defined by an infinite number of indefinite quadratic constraints (which in addition also are non-linear in $\mathbf{x}$).

4 Necessary and Sufficient Conditions for Bijectivity

Given the complexity of the set of bijective thin-plate spline deformations, the task finding a defining expression for it analytically is a formidable one. One approach could for instance be to try and solve the envelope [3] equations

$$\mathbf{Y}^T B_{\mathbf{T}}(\mathbf{x}) \mathbf{Y} = 0 \quad (10)$$

$$\mathbf{Y}^T B(x)_{\mathbf{T}}(\mathbf{x})'_{x_1} \mathbf{Y} = 0 \quad (11)$$

$$\mathbf{Y}^T B(x)_{\mathbf{T}}(\mathbf{x})'_{x_2} \mathbf{Y} = 0 \quad (12)$$

It can be shown that since the constrain tangents $\Omega_{\mathbf{T}}^+$ at its boundary $\partial\Omega_{\mathbf{T}}^+$, the points on $\partial\Omega_{\mathbf{T}}^+$ is a subset of the envelope of the family of all the quadratic functions.

Instead we have chosen to use numerical methods to derive conditions on $\Omega_{\mathbf{T}}^+$. By finding the minimum-volume ellipsoid E_1 covering $\Omega_{\mathbf{T}}^+$ and the maximum-volume ellipsoid E_2 inscribed in $\Omega_{\mathbf{T}}^+$ we obtain a necessary and a sufficient conditions on $\mathbf{Y}$. That is

$$\mathbf{Y} \notin E_1 \Rightarrow \mathbf{Y} \notin \Omega_{\mathbf{T}}^+ \quad (13)$$

$$\mathbf{Y} \in E_2 \Rightarrow \mathbf{Y} \in \Omega_{\mathbf{T}}^+ \quad (14)$$

Finding such extremal volume ellipsoids can be formulated as optimization problems [4, 5]. But since we have finitely many variables and infinite number of constraints we have a semi-infinite program on our hand [7]. In order to avoid this we simply approximate $\Omega_{\mathbf{T}}^+$ by the intersection of a finite subset of these constraints.

$$\tilde{\Omega}_{\mathbf{T}}^+ = \{\mathbf{Y} \in \mathbb{R}^{2k} \mid \hat{\mathbf{Y}}^T B_{\mathbf{T}}(\mathbf{x}) \hat{\mathbf{Y}} > 0, \\ \text{for a finite number of } \mathbf{x} \in \mathbb{R}^2\}$$

With E_1 and E_2 defined by $E_i = \{p \in \mathbb{R}^n \mid p^T A_i p + 2b_i^T p + c_i \geq 0\}$ and the bijectivity constraints in the form $\{Y \in \mathbb{R}^n \mid Y^T F(\mathbf{x}) Y + 2g^T Y + h(\mathbf{x}) \geq 0\}$ we proceed.

The minimum volume ellipsoid is always a convex optimization problem regardless the set it covers. Using the introduced notation. E_1 will be the solution to the following convex program

$$\begin{aligned} & \text{minimize } -\log \det E_1 \\ & \text{s.t. } \begin{bmatrix} A_1 - \sum \tau_i F(\mathbf{x}_i) & A_1 b_1 - \sum \tau_i g(\mathbf{x}_i) \\ (A_1 b_1 - \sum \tau_i g(\mathbf{x}_i))^T & c_1 - \sum \tau_i h(\mathbf{x}_i) \end{bmatrix} \succeq 0 \end{aligned}$$

The maximum volume inscribed ellipsoid is a convex optimization problem if the covering set itself is convex. Since $\Omega_{\mathbf{T}}^+$ in general is non-convex

Figure 5: Example of a subset of $\Omega_{\mathbf{T}}^+$ (corresponding to letting $\mathbf{Y}$ free in two dimensions).

Figure 6: Example of necessary (larger ellipsoid) and sufficient conditions (smaller ellipsoid) on the same subset as above.

we must employ other optimization algorithms. Nevertheless, E_2 will be the solution to the following optimization problem

$$\begin{aligned} & \text{maximize } -\log \det E_2 \\ \text{s.t. } & \begin{bmatrix} F(\mathbf{x}_i) - A_2 & g(\mathbf{x}_i) - A_2 b_2 \\ (g(\mathbf{x}_i) - A_2 b_2)^T & h(\mathbf{x}_i) - c_i \end{bmatrix} \succeq 0 \end{aligned}$$

5 Conclusion and Future Work

Even though this paper very much describes a work in progress, it does contain a formulation of how to characterize the set of bijective thin-plate splines. It also includes a discussion of some experimentally derived indications of some other properties of this set as well as a method for finding necessary and sufficient conditions for bijectivity. Future work includes finding such conditions analytically as well as attempting to prove its convexity and boundedness properties.

References

- [1] F. L. Bookstein, "Principal Warps: Thin-Plate Splines and the Decomposition of Deformations", IEEE trans. Pattern Analysis and Machine Intelligence, Vol. 11, No. 6, 1989.

- [2] Kent J. T. and Mardia K. V., "The link between kriging and thin-plate splines.", Probability, statistics and Optimization: a Tribute to Peter Whittle, p325-329.
- [3] Bruce J.W. and Giblin P.J., "Curves and Singularities", Cambridge University Press.
- [4] Vandenberghe L. and Boyd S., "Convex Optimization", Cambridge University Press.
- [5] Vandenberghe L., Boyd S. and Wu S.W., "Determinant Maximization with Linear Matrix Inequality Constraints", SIAM Journal on Matrix Analysis and Applications, Volume 19, Number 2, pp. 499-533.
- [6] Vandenberghe L. and Boyd S., "Semidefinite Programming", SIAM Review, Volume 38, Number 1, pp. 49-95.
- [7] Hettich R. and Kortanek K.O., "Semi-infinite programming: theory, methods, and applications", SIAM Review, Volume 35, Number 3, pp. 380-429.