Simplifying Transformations for a Family of Elastic Metrics on the Space of Surfaces

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Abstract

We define a new representation for immersed surfaces in $\mathbb{R}^3$ by combining the SRNF and the induced surface metric. Using the L^2 metric on the space of SRNFs and the DeWitt metric on the space of surface metrics, we obtain a 3-parameter family of metrics that corresponds to the family of "elastic metrics" proposed by Jermyn et al. in [19] on the space of immersed surfaces. Similar to the original SRNF representation this new representation results in an extrinsic distance function on the space of immersed surfaces that is easy to compute as it is given by an explicit formula. In addition to avoiding the degeneracy of the SRNF it allows for a data-driven choice of the parameters of the metric, while still providing for fast and accurate registration of surfaces.

1. Introduction

Shape analysis of surfaces plays an important role in many applications such as anatomy, bioinformatics, computer graphics, computer vision, and medical imaging [25, 2, 17, 18, 34]. The main goals in this area are to quantify the difference between the shapes of two surfaces and to conduct statistical analyses on the space of shapes. If, as in this paper, we assume that our surfaces are given in parametrized form, the main challenge is to remove the effects of shape-preserving transformations, which consist of reparametrizations and/or rigid motions.

The problem of removing the effects of reparametrizations can be thought of as a registration problem, i.e., finding the optimal point-correspondence between two surfaces. This problem is challenging because it is an optimization problem over the infinite-dimensional group of reparametrizations. In previous work, this problem was often solved by a 2-step process, in which the two surfaces first were registered using one criterion, while deformations and distances were then computed independently using a different criterion [2, 6, 16, 29, 12, 18, 22]. However, because of the different sets of criteria, this approach can lead to undesirable statistical biases and make the overall analysis suboptimal [31].

Elastic shape analysis is an approach in which the determination of optimal point correspondences and optimal deformations is accomplished by a single criterion. The main idea is to equip the space of parametrized surfaces with a Riemannian metric that is invariant under the group of all relevant shape-preserving transformations. This metric then induces a metric on the quotient space ("shape space") under this group, and geodesics and distances on the shape space are defined using this induced metric.

In recent years several metrics and frameworks [19, 27, 26, 3, 31, 35, 32, 33, 4, 5] have been introduced for the study of elastic shape analysis. In [19], Jermyn et al. proposed a family of metrics, called the "general elastic metric" for surfaces in $\mathbb{R}^3$, which is a generalization of a previously studied family of elastic metrics on the space of curves [28]. It is defined as a weighted sum of three components that measure changes in shearing, stretching and bending of the surface. In the same paper [19], motivated by the SRVF framework for comparing curves [31], Jermyn et al. introduced the Square Root Normal Fields (SRNF) for comparing shapes of surfaces. In this method, a map is defined from the space of parametrized surfaces to an L^2 space, and the pullback of the L^2 metric under this map is shown to be one member of the family of general elastic metrics, albeit a degenerate member, in which one of the three coefficients vanishes. The SRNF framework has proven efficient and successful in many applications [27, 20, 21, 24]. However, the degeneracy creates serious problems; for example, there exist pairs of surfaces with different shapes having exactly the same SRNF (so their SRNF distance vanishes) [23]. In fact, the SRNF map is neither injective nor surjective and

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its image is not fully understood. In [27], appealing deformations of surfaces are produced by producing numerical approximations to the inverse of the SRNF map along straight lines in the L^2 space. Of course, geodesics in the L^2 image space are straight lines, but these straight lines generally leave the image of the SRNF map and thus the resulting deformations are not geodesics.

In [32], Su et al. proposed a 4-parameter family of metrics on the space of parametrized surfaces which has the desired invariance properties. This 4-parameter family contains the 3-parameter general elastic metrics as a special case. Most of the metrics in this family are not degenerate and geodesics and distances in shape space can be computed numerically. The drawback of this method is that computationally it is not as fast as the SRNF representation.

Contributions of this article: The purpose of this article is to introduce a new representation for surfaces by combining the SRNF map with a direct consideration of the Riemannian metric on the parametrized surface induced by its immersion into $\mathbb{R}^3$. By endowing the space of SRNFs with the L^2 metric and the space of metrics with the DeWitt metric, the pullback of the product metric gives an open subset of the 3-parameter family of the general elastic metrics. In addition, there are explicit formulas for minimal geodesics and for the geodesic distance function in the image space, which make the matching of surfaces computationally efficient. This new representation is injective but not surjective. Thus our new method overcomes the degeneracy of the SRNF-method, but similarly to the SRNF, the geodesics in the image space do leave the image of the space of surfaces. For this reason, the method given in this article does not provide a computation of actual geodesics with respect to this family of metrics. The main uses of this article are (1) to efficiently calculate a first-order approximation of geodesic distance, and (2) to provide an effective method of registering two surfaces, thereby yielding a good initialization for the methods of [32].

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2. The Space of Shapes

For the purpose of this article we model all parametrized surfaces as immersions from a two dimensional compact, smooth manifold M with a possible boundary to $\mathbb{R}^3$, i.e., smooth maps from M to $\mathbb{R}^3$ with injective tangent mappings. Denote by $\operatorname{Imm}(M,\mathbb{R}^3)$ the space of immersions and $\mathcal{G}$ the group of shape-preserving transformations. Then the "shape space" of surfaces is a quotient space

$$\mathcal{S}(M,\mathbb{R}^3) = \operatorname{Imm}(M,\mathbb{R}^3)/\mathcal{G},$$

where $\mathcal{G} = \operatorname{Diff}_+(M)$ or $\mathcal{G} = \operatorname{Diff}_+(M) \times \operatorname{SO}(3) \ltimes \mathbb{R}^3$ depending on different applications. Here the group of orientation-preserving diffeomorphisms $\operatorname{Diff}_+(M)$ acts on the space of immersions $\operatorname{Imm}(M,\mathbb{R}^3)$ by right composition $(f,\gamma) \mapsto f \circ \gamma$; the group of rigid motions, given by the semidirect product $\operatorname{SO}(3) \ltimes \mathbb{R}^3$ of the group of rotations $\operatorname{SO}(3)$ and the group of translations $\mathbb{R}^3$, acts on the space of immersions $\operatorname{Imm}(M,\mathbb{R}^3)$ according to $((R,v),f) \mapsto Rf + v$. Two surfaces will be considered to have the same shape if they are in the same orbit under the action of the group $\mathcal{G}$.

The shape space $\mathcal{S}(M,\mathbb{R}^3)$ is not a smooth manifold but only an orbifold [10]. However, we will ignore these subtleties and assume that we are working away from the singularities. To study the space of shapes, we will put a Riemannian metric on the space of immersions $\operatorname{Imm}(M,\mathbb{R}^3)$ that is invariant under the action of $\mathcal{G}$. Then this Riemannian metric on $\operatorname{Imm}(M,\mathbb{R}^3)$ induces a Riemannian metric on the shape space $\mathcal{S}(M,\mathbb{R}^3)$ and makes it - via the geodesic distance function - into a metric space. It thus enables us to calculate geodesics and geodesic distance and conduct statistical analysis on the shape space $\mathcal{S}(M,\mathbb{R}^3)$.

Denote by d_{Imm} the distance function with respect to the Riemannian metric on $\operatorname{Imm}(M,\mathbb{R}^3)$. Let $[f]$ be the equivalence class of $f \in \operatorname{Imm}(M,\mathbb{R}^3)$ under the action of $\mathcal{G}$. Then given two surfaces $f_1, f_2 \in \operatorname{Imm}(M,\mathbb{R}^3)$, the distance function on $\mathcal{S}(M,\mathbb{R}^3)$ is given by

$$d_{\mathcal{S}}([f_1],[f_2]) = \inf_{\gamma\in\operatorname{Diff}_+(M)} d_{\operatorname{Imm}}(f_1\circ\gamma, f_2)$$

if $\mathcal{G} = \operatorname{Diff}_+(M)$ and

$$d_{\mathcal{S}}([f_1],[f_2]) = \inf_{\substack{\gamma\in\operatorname{Diff}_+(M)\\ R\in\operatorname{SO}(3), v\in\mathbb{R}^3}} d_{\operatorname{Imm}}(f_1\circ\gamma, Rf_2+v)$$

if $\mathcal{G} = \operatorname{Diff}_+(M) \times \operatorname{SO}(3) \ltimes \mathbb{R}^3$. To calculate the distance between two shapes, we will need to find an element in $\mathcal{G}$ that realizes the infimum on the right side if it is realized, or at least approximates it if the infimum is not realized.

2.1. The Elastic Metric on the Space of Surfaces

Jermyn et al. in [19] introduced a 3-parameter family of metrics on the space of surfaces, which is invariant under the action of the group of diffeomorphisms and the action of the group of rigid motions. This 3-parameter family of metrics is called the general elastic metric. To define this family of metrics, we first introduce the (g,n) representation for surfaces. Let (u,v) be local coordinates on M. It is well known, see e.g. [1], that (up to translation) each surface f has a unique (g,n) representation, where g is the Riemannian metric on M induced by f and $n = \frac{f_u\times f_v}{|f_u\times f_v|}$ is the unit normal vector field to the surface f. Using this (g,n) representation, the general elastic metric is given as follows:

$$
\begin{aligned}
&G_{(g,n)}\left((\delta g,\delta n),(\delta g,\delta n)\right) \qquad (1)\\
=&a\int_M \operatorname{tr}\left(g^{-1}\delta g_0 g^{-1}\delta g_0\right)\mu_g + b\int_M \left(\operatorname{tr}\left(g^{-1}\delta g\right)\right)^2\mu_g\\
&\quad + c\int_M \langle \delta n,\delta n\rangle_{\mathbb{R}^3}\mu_g,
\end{aligned}
$$

where $a, b, c \geq 0$ and μ_g is the induced volume form of the surface f. The first term in formula (1) measures the area-preserving change in metric, the second term measures the change in area and the last term measures the change of the normal direction. However, this 3-parameter family of metrics was not used for comparing surfaces. Instead, Jermyn et al. [19] proposed the Square Root Normal Field (SRNF) representation of surfaces and used the L^2 metric on the space of SRNFs, which corresponds to a special case of the general elastic metric, for shape analysis of surfaces. We will give more detail about the SRNF representation in Section 3.1.

3. A Simplifying Transformation

In this section we will introduce a new transformation that will lead to efficient algorithms for the 3-parameter family of elastic metrics (1); similarly to the SRNF-representation, the new representation will provide a first-order approximation of the geodesic distance with respect to more general members of the family of elastic metrics (instead of just the single degenerate case that is handled by the SRNF). Before we propose the new representation, we will describe the SRNF representation in more detail and describe an important one-parameter family of metrics on the space of all Riemannian metrics.

3.1. The SRNF Representation

The SRNF representation, proposed by Jermyn et al. [19], is a map given by

$$
\begin{aligned}
\operatorname{Imm}(M,\mathbb{R}^3) &\to C^\infty(M,\mathbb{R}^3) \qquad (2)\\
f(s) &\mapsto \sqrt{A(s)}\, n(s),
\end{aligned}
$$

where $A(s) = |f_u \times f_v|$ is the area measure induced by f and n is the unit normal vector field to the surface f. The motivation for this transformation is given by the observation that the pullback of the L^2 metric on the target space $C^\infty(M,\mathbb{R}^3)$ is the general elastic metric (1) for $a = 0, b = \frac{1}{16}, c = 1$ on the space of immersions $\operatorname{Imm}(M,\mathbb{R}^3)$, see [19]. The geodesic distance of the L^2 (Riemannian) metric on $C^\infty(M,\mathbb{R}^3)$ is simply the L^2 norm of the difference between the given two functions and thus this framework presents an extremely efficient approximation of the geodesic distance of the corresponding elastic metric on the space of surfaces. Note that it is only an approximation of the geodesic distance, since the linear path between two SRNFs will, in general, leave the image of the SRNF map. Thus the resulting distance should be viewed as an extrinsic distance obtained by embedding the space of parametrized surfaces in a linear space. Furthermore the pullback metric consists only of the last two terms of the general elastic metric (1), thus it is degenerate: in the recent paper [23] the authors describe several examples of pairs of surfaces with different geometric features for which the SRNF distance vanishes.

3.2. The DeWitt Metric on the Space of Metrics

In this section we will describe the second main ingredient for the proposed transformation, a family of reparametrization invariant Riemannian metrics on the space of all Riemannian metrics, often referred to as DeWitt or (for a special choice of constant) Ebin metric. A Riemannian metric on M is a smooth, positive definite symmetric $(0,2)$ tensor field on M. The space of all Riemannian metrics $\operatorname{Met}(M)$ is thus the set of all smooth, positive definite symmetric $(0,2)$ tensor fields on M, which is an infinite dimensional manifold [14]. The tangent space at each point in $\operatorname{Met}(M)$ is the space of all smooth, symmetric $(0,2)$ tensor fields. In local coordinates, a metric g can be represented as a field of 2×2 positive definite symmetric matrices that vary smoothly over M and every tangent vector at g can be represented as a field of symmetric matrices.

The DeWitt (or Ebin) metric is a one parameter family of metrics defined on the space of metrics $\operatorname{Met}(M)$. It has been introduced in [13] and studied in detail in [15]. For $g \in \operatorname{Met}(M)$ and $\delta g \in T_g\operatorname{Met}(M)$ this family of metrics is defined as

$$
\begin{aligned}
&G_g^\lambda(\delta g,\delta g) \qquad (3)\\
&\quad= \int_M \left(\operatorname{tr}\left(g^{-1}\delta g_0 g^{-1}\delta g_0\right) + \lambda\left(\operatorname{tr}(g^{-1}\delta g)\right)^2\right)\mu_g,
\end{aligned}
$$

where $\lambda > 0$, $\delta g_0 = \delta g - \frac{1}{2}\operatorname{tr}(g^{-1}\delta g)g$ is called the traceless part of δg and μ_g is the volume form on M induced by g. To understand better the geometric meaning of this family of metrics we take a closer look at the purpose of the two terms in the metric: using the variational formula of the volume form of a Riemannian metric it is easy to see that second term measures exactly the change in the volume form, while the first term measures the change in the metric within a family of metrics with the same volume form. This family of metrics is a generalization of the Ebin metric [14], which is given by the metric (3) for $\lambda = \frac{1}{\dim(M)} = \frac{1}{2}$.

In the following, we consider the action of the group of diffeomorphisms $\operatorname{Diff}_+(M)$ on $\operatorname{Met}(M)$ by pullbacks:

$$
\begin{aligned}
\operatorname{Met}(M)\times\operatorname{Diff}_+(M) &\to \operatorname{Met}(M) \qquad (4)\\
(g,\varphi) &\mapsto \varphi^* g = d\varphi^T g(\varphi) d\varphi.
\end{aligned}
$$

The following theorem shows the invariance under this action of the family of metrics (3), which guarantees that the metric is independent of choice of local coordinates on M. The proof of this result follows immediately from Theorem 5 in Appendix A and the transformation formula for multi-dimensional integrals. (This theorem is also an immediate consequence of DeWitt's original paper on this metric [13].)

Theorem 1. *Let $g \in \operatorname{Met}(M)$ and $\delta g \in T_g \operatorname{Met}(M)$. Then the DeWitt metric (3) is invariant under the action (4) of the group of diffeomorphisms $\operatorname{Diff}_+(M)$, i.e., let $\varphi \in \operatorname{Diff}_+(M)$ we have*

$$G^\lambda_{\varphi^* g}(\varphi^*\delta g, \varphi^*\delta g) = G^\lambda_g(\delta g, \delta g).$$

For most Riemannian metrics on infinite dimensional manifolds, calculating geodesics and geodesic distance is a challenging task that can usually only be solved approximately by (numerically) minimizing a discretized version of the energy functional. The beauty of the DeWitt metrics (3) lies in the observation that they are pointwise metrics, i.e. they can be written as integrals of Riemannian metrics on the space of positive definite, symmetric 2×2-matrices. By the results of [9] this enables us to reduce the study to the study of the corresponding metric on the space of positive definite symmetric 2×2 matrices, We will present some results of the induced geometry on the space of positive definite symmetric matrices in Appendix A. These results will allow us to obtain explicit formulas for geodesics on the space $\operatorname{Met}(M)$, which are given for each $x \in M$ by the geodesic formula in Theorem 6 on the space of positive definite symmetric matrices in Appendix A.

For the purpose of this article, we are mainly interested in the formula for the induced geodesic distance. The space of metrics $\operatorname{Met}(M)$ with respect to the geodesic distance of the DeWitt metric is not metrically complete for any choice of λ. However, following the analysis of Clarke [11] for the Ebin metric, we can determine the metric completion of $\operatorname{Met}(M)$ for any choice of λ, denoted in the following by $\overline{\operatorname{Met}}(M)$, which is given by $\widetilde{\operatorname{Met}}(M)/\sim$. Here $\widetilde{\operatorname{Met}}(M)$ is the space of all semi-metrics on M, i.e., the space of all measurable, positive semi-definite symmetric $(0,2)$ tensor fields on M, and the equivalence relation $\sim$ is defined via $g_1 \sim g_2$ if the statement

$$g_1(x) \neq g_2(x) \iff g_1(x) \text{ and } g_2(x) \text{ both are degenerate}$$

holds almost everywhere on M.

The following theorem, in which we present an explicit formula for the distance function on the metric completion $\overline{\operatorname{Met}}(M)$, will be essential for the construction of our family of transformations.

Theorem 2. *Let $g_1, g_2 \in \overline{\operatorname{Met}}(M)$. Then the square of the geodesic distance for the family of metrics (3) is*

$$d^\lambda(g_1, g_2)^2 = \int_M d^\lambda_{\text{Sym}}(g_1(x), g_2(x))^2\, dx, \tag{5}$$

where

$$d^\lambda_{\text{Sym}}(g_1(x), g_2(x))^2 = 16\lambda\left(s_1^2(x) - 2 s_1(x) s_2(x)\cos(\theta(x)) + s_2^2(x)\right),$$

with

$$s_1(x) = \sqrt[4]{\det(g_1(x))}, \quad s_2(x) = \sqrt[4]{\det(g_2(x))},$$
$$\theta(x) = \min\left\{\pi, \frac{\sqrt{\lambda^{-1}\operatorname{tr}(K_0^2(x))}}{4}\right\},$$
$$K(x) = \begin{cases} 0 & \text{if either } g_1(x) \text{ or } g_2(x) \text{ is degenerate} \\ g_1(x)\log(g_1(x)^{-1}g_2(x)) & \text{else.}\end{cases}$$
$$K_0(x) = K(x) - \operatorname{tr}(g_1^{-1}(x)K(x))g_1(x).$$

Proof. This result is a generalization of the result given by Clarke in [11] for the standard Ebin metric. The details of this proof would exceed the page limits of this article; instead, we refer the interested reader to [15] which contains the most important ingredients and allows us to generalize the results of Clarke. □

3.3. The (g, q) Representation

In the following we will present a new family of transformations by considering both the induced surface (Riemannian) metric and the SRNF of the surface. Note that using the (g, n) representation, we could obtain the whole 3-parameter family of the elastic metrics (1). However, there exists no explicit formula for geodesics (geodesic distance resp.) under this representation and thus this (g, n) representation is not a good choice for our purposes.

Motivated by the results of the previous two subsections, we consider the (g, q) representation for a surface, where g is the metric induced by the surface and q is the SRNF of the surface, i.e., we consider the map

$$\mathcal{Q} : \operatorname{Imm}(M, \mathbb{R}^3)/\mathbb{R}^3 \to \operatorname{Met}(M) \times C^\infty(M, \mathbb{R}^3)$$
$$f \mapsto (g, q),$$

where the $\mathbb{R}^3$ being modded out by denotes the group of translations, $g = df^T df$ and $q(s) = \sqrt{A(s)}n(s)$ with df being the differential of f and $A(s)$ and $n(s)$ as in (2). It follows from the uniqueness (up to translations) of the (g, n) representation [1] that the map $\mathcal{Q}$ is injective.

Let $(g, q) \in \operatorname{Met}(M) \times C^\infty(M, \mathbb{R}^3)$ and $(\delta g, \delta q) \in T_g \operatorname{Met}(M) \times T_q C^\infty(M, \mathbb{R}^3)$. In the following we will define a 3-parameter family of Riemannian metrics on the product space $\operatorname{Met}(M) \times C^\infty(M, \mathbb{R}^3)$ as follows

$$G^{\alpha,\beta,\lambda}_{(g,q)}\left((\delta g, \delta q), (\delta g, \delta q)\right) = \alpha G^\lambda(\delta g, \delta g) + \beta \langle \delta q, \delta q\rangle_{L^2}, \tag{6}$$

where $\alpha, \beta > 0$, G^λ is the family of metrics on $\operatorname{Met}(M)$ given by (3) and $\langle \cdot, \cdot \rangle_{L^2}$ denotes the L^2 inner product on $C^\infty(M, \mathbb{R}^3)$. The following theorem, which constitutes the first of our main results, connects this family of new Riemannian metrics to the general elastic metric:

Theorem 3. *The pullback of the family of metrics* (6) *on the space* $\operatorname{Imm}(M, \mathbb{R}^3)$ *under the map* $\mathcal{Q}$ *is the general elastic metric as introduced in* (1) *with* $a = \alpha$, $b = \alpha\lambda + \frac{\beta}{16}$ *and* $c = \beta$.

Proof. Using that the pullback of the L^2 metric gives the general elastic metric for $a = 0, b = \frac{1}{16}, c = 1$, the proof of this result is straightforward. □

Note that we have thus constructed a transformation for the 3-parameter family of elastic metrics (1) for all choices of coefficients with $a > 0, b > \frac{c}{16}, c > 0$. The main reason for introducing this particular representation will become clear in the next theorem, which will provide us with a first order approximation of the geodesic distance on the space of immersions. Let d_{Imm} be the pullback via $\mathcal{Q}$ of the geodesic distance on the product space $\operatorname{Met}(M) \times C^\infty(M, \mathbb{R}^3)$. Then d_{Imm} is reparametrization invariant. The following theorem provides an explicit formula for it:

Theorem 4. *Let* $f_1, f_2 \in \operatorname{Imm}(M, \mathbb{R}^3)$ *and*

$$(g_1, q_1) = \mathcal{Q}(f_1), \quad (g_2, q_2) = \mathcal{Q}(f_2).$$

Then the square of the distance d_{Imm} *between* f_1 *and* f_2 *is given by*

$$d_{\mathrm{Imm}}(f_1, f_2)^2 = \alpha d^\lambda(g_1, g_2)^2 + \beta \left\| q_1 - q_2 \right\|^2_{L^2}, \tag{7}$$

where d^λ *is given by* (5) *and* $\|\cdot\|_{L^2}$ *denotes the* L^2 *norm on* $C^\infty(M, \mathbb{R}^3)$.

Note that the map $\mathcal{Q}$ is not surjective and the image of the representation is not totally geodesic. Thus the geodesics in the product space $\operatorname{Met}(M) \times C^\infty(M, \mathbb{R}^3)$ will leave the image of the space of immersions and the distance d_{Imm} only gives an approximation to the geodesic distance between surfaces. Similar to the SRNF representation, there is also no explicit formula for the inverse of this (g, q) representation. However, an advantage of this new (g, q) representation for shape analysis of surfaces is the fact that the map $\mathcal{Q}$ is injective. Like the (g, n) representation, it yields a family of non-degenerate elastic metrics. In addition, we have explicit formulas for the minimal geodesics and the geodesic distance function in the image space, which makes the matching between two surfaces computationally efficient.

4. Optimization Over Shape Preserving Transformations

In this section we present the resulting optimization procedure for solving the registration problem in the newly proposed framework. For the presentation in this section we will assume that $M = S^2$, which allows us to parametrize any surface using spherical coordinates $(\theta, \phi) \in [0, 2\pi] \times [0, \pi]$, where θ denotes the azimuthal angle and ϕ denotes the polar angle. For the construction of such a parametrization we refer to the articles [30, 26].

Given two surfaces $f_1, f_2 \in \operatorname{Imm}(M, \mathbb{R}^3)$ we aim to find the optimal point correspondence between the shapes of these two surfaces, i.e. we want to find the optimal $\gamma \in \operatorname{Diff}_+(S^2)$ that realizes the following infimum

$$d_{\mathcal{S}}([f_1], [f_2])^2 = \inf_{\gamma \in \operatorname{Diff}_+(S^2)} d_{\mathrm{Imm}}(f_1 \circ \gamma, f_2)^2,$$

where $[f_1]$ and $[f_2]$ are the equivalence classes of f_1 and f_2 under the action of the group of diffeomorphisms $\operatorname{Diff}_+(S^2)$, respectively, and the distance function d_{Imm} is given by formula (7). Note that, in general, the existence of optimal reparametrizations is not guaranteed, see e.g. [8]. We observed however a good and stable convergence behavior of our numerical algorithms.

In the following let Id be the identity map from S^2 to itself and let $\{v_i, i = 1, \cdots, L\}$ be a truncated orthogonal basis for the space of all smooth tangent vector fields on S^2 with respect to the Euclidean metric, see e.g. [32] on how to construct such a basis. We then define

$$\gamma = \operatorname{Proj}\left(\mathrm{Id} + \sum_{i=1}^{L} X^i v_i\right), \tag{8}$$

where Proj is the projection map from $\mathbb{R}^3$ to the unit sphere S^2. The resulting mapping γ is a diffeomorphism of S^2 if the size of the coefficient vector $X = (X^1, X^2, \cdots, X^L)$ is small enough, see [32, Theorem 3]. We are aiming to minimize the functional $F : \mathbb{R}^L \to \mathbb{R}$ given by

$$F(X) = d_{\mathrm{Imm}}(f_1 \circ \gamma, f_2)^2,$$

where γ is of the form (8). To find the best coefficient vector $X = (X^1, X^2, \cdots, X^L)$ we employ a BFGS method as provided in the optimize package of scipy with the gradient calculated using automatic differentiation in Pytorch. Since the maps obtained by formula (8) only lead to 'small' deformations we iterate this optimization procedure. Like any gradient based method it is important to choose a good initialization for our BFGS method. For this purpose, we use the icosahedral group, which contains 60 orientation preserving rotations, and can be viewed as a discrete subset of the diffeomorphism group of S^2. We use as our initial guess the element of the icosahedral group that minimizes the distance.

We will now describe how one can deal with other shape preserving group actions, i.e., translations and rotations. Our family of metrics (6) is naturally defined on the quotient space of surfaces modulo translations, as translations (constant vector fields) form exactly the kernel of our metric. Therefore to solve the registration problem on the space of unparametrized sufaces modulo rigid motions it remains to minimize over the group of rotations, i.e. we need to solve a joint optimization problem of finding the optimal $\gamma \in \operatorname{Diff}_+(S^2)$ and $R \in \mathrm{SO}(3)$ that realize

$$d_{\mathcal{S}}([f_1],[f_2])^2 = \inf_{\substack{\gamma\in \operatorname{Diff}_+(S^2)\\ R\in\mathrm{SO}(3)}} d_{\mathrm{Imm}}(f_1\circ\gamma, Rf_2)^2,$$

where $[f_1]$ and $[f_2]$ are the equivalence classes of f_1 and f_2 under the actions of the group of diffeomorphisms $\operatorname{Diff}_+(S^2)$ and the group of rotations $\mathrm{SO}(3)$. We use a similar approach as we discussed before to solve this joint optimization problem and we omit the details here.

Remark 1. *The framework developed in [32] for calculating geodesics with respect to the* 4*-parameter family of elastic metrics could be used here for calculating geodesics with respect to the new family of metrics* (6) *both in the space of unparametrized surfaces and in the space of unparametrized surfaces modulo rigid motions. This is based on the following correspondence: the pullback of the metric* (6) *gives the* 4*-parameter family of metrics for* $\mathfrak{a} = 4\alpha, \mathfrak{b} = 8\alpha\lambda + \beta/2, \mathfrak{c} = \beta, \mathfrak{d} = 0$. *Therefore, the geodesics could be calculated after solving the registration problem first using this new* (g, q) *representation. We expect this procedure to lead to a significant speed-up over the algorithm of [32].*

5. Numerical Experiments

In this section, we will present numerical results to validate our proposed method for surface matching. To better visualize the obtained registrations we will also depict the corresponding geodesics, which are calculated using the framework developed in [32] where the point registrations are obtained from the present implementation, cf. Remark 1.

In Figure 1 we consider a pair of parametrized spherical surfaces with one bump on different positions. The parametrization of the surface is visualized by the color map of the surface. The initial and final correspondences between this pair of surfaces for the general elastic metric (1) with different constants are depicted. One can clearly see the effect of the constants a, b, c on the resulting surface registrations. To better visualize the resulting point correspondences we depict the corresponding geodesics between these pairs of surfaces in Figure 2: In the first row the bump on the first surface is shrunk and a new bump is grown out on the correct location. If we decrease the weight that measures the change in the metric then the bump on the target shape corresponds to the bump on the initial shape and the target shape is obtained by shearing the neighborhood of the initial bump, which can be seen in the second row. In the last row, where we put only a small weight on measuring the change of normal directions, the bump is simply moving (sliding) along the surface to its new position. This experiment suggests that one can model a variety of different behaviors by appropriately choosing the constants. Similar effects can be observed in our second toy example where we consider a pair of spherical surfaces with two bumps at different locations, cf. Figure 3. Finally in Figure 4 we show an example of surface matching using real data from the SHREC07 watertight models database [7], where the initial parametrizations of the boundary surfaces are obtained using the code from [26]. All results were obtained on a standard laptop with 16 basis elements for the space of tangent vector fields on S2. With this setup all each of our experiments was computed in less than 10 seconds.

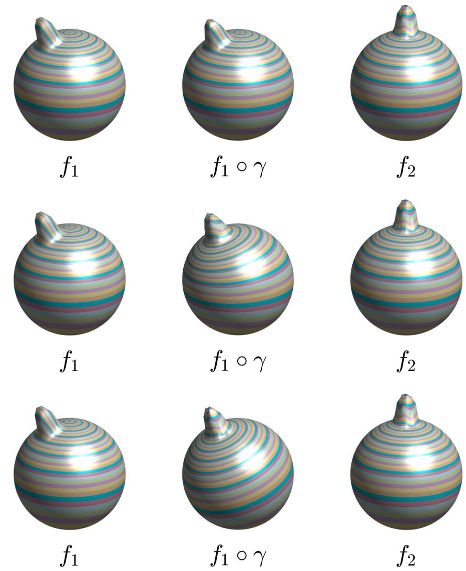

Figure 1. Matchings between surfaces with one bump in the space of unparametrized surfaces $\mathrm{Imm}(S^2, \mathbb{R}^3)/\operatorname{Diff}_+(S^2)$ with respect to the general elastic metric (1) for $a = 0.1, b = 0.07, c = 1$ (first row), $a = 0.01, b = 0.07, c = 1$ (second row) and $a = 1, b = 1, c = 0.1$ (third row). In each row, the surfaces on the left and right show the original parametrizations of the boundary surfaces; the second one gives the final parametrization of the first boundary surface after the whole optimization process.

6. Conclusion

In this paper we have introduced a new representation for immersed surfaces in $\mathbb{R}^3$ by considering both the induced metric and the SRNF of each surface. By endowing the space of metrics with the DeWitt metric and the space of SRNFs with the L^2 metric, we have obtained an open subset of the 3-parameter family of elastic metrics intro-

Figure 2. Geodesics between surfaces with one bump in the space of unparametrized surfaces $\mathrm{Imm}(S^2, \mathbb{R}^3)/\,\mathrm{Diff}_+(S^2)$ with respect to the general elastic metric (1) for $a = 0.1, b = 0.07, c = 1$ (first row), $a = 0.01, b = 0.07, c = 1$ (second row) and $a = 1, b = 1, c = 0.1$ (third row). Here each geodesic is calculated with the method provided in [32] using the final point correspondence of our new algorithm.

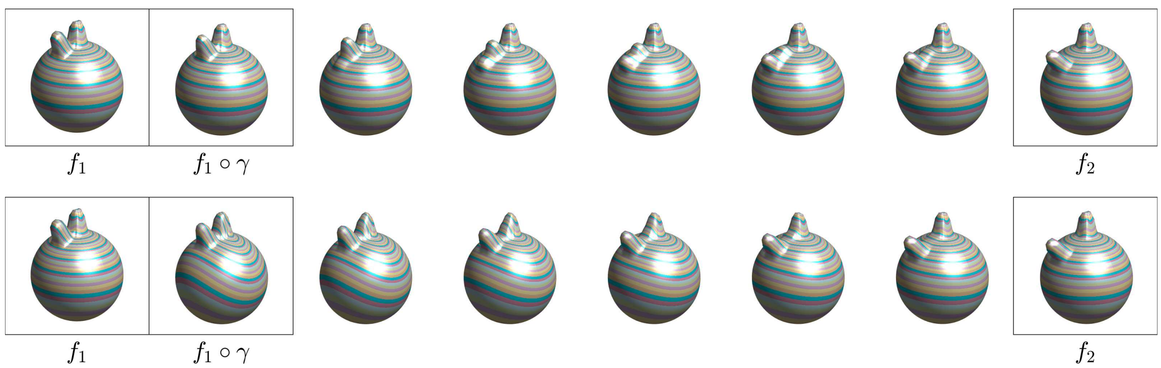

Figure 3. The matchings and geodesics between surfaces with two bumps in the space of unparametrized surfaces $\mathrm{Imm}(S^2, \mathbb{R}^3)/\,\mathrm{Diff}_+(S^2)$ with respect to the general elastic metric (1) for $a = 1, b = 1, c = 1$ (first row) and $a = 0.1, b = 1, c = 1$ (second row). In each row, the surface f_1 on the left and f_2 on the right show the original parametrizations of the boundary surfaces; the second one $f_1 \circ \gamma$ gives the final parametrization of the first boundary surface after the whole optimization process; the right 7 surfaces on the right show the interpolating geodesic. Here each geodesic is calculated with the method provided in [32] using the final point correspondence of our new algorithm.

duced by Jermyn et al. in [19]. Compared to the SRNF representation, the advantage of using this new representation is that it leads to a whole family of non-degenerate elastic metrics, which enables us to choose the constants in a data-driven way. Additionally, it yields explicit formulas for minimal geodesics and for the geodesic distance function in the image space, which makes the matching between surfaces computationally efficient. Similar to the SRNF, the geodesic in the image space might leave the image of the space of surfaces. Although in this situation the method does not provide the actual geodesics between shapes, it still yields an effective method to register surfaces. We have presented several examples of registration between surfaces to validate our framework.

In future work we plan to apply our algorithms to real data sets to further investigate the influence of the constants and to generalize this new representation such that it allows to represent the whole family of elastic metrics by considering the pseudo-Riemannian DeWitt metric on the space of metrics where the constant λ can be negative.

A. The Space of Positive Definite Symmetric $n \times n$ Matrices

Denote by $\mathrm{Sym}_+(n)$ the space of positive definite symmetric $n \times n$ matrices. The space $\mathrm{Sym}_+(n)$ is an open subset of the space of all $n \times n$ symmetric matrices, denoted by $\mathrm{Sym}(n)$. Thus it is a manifold of dimension $\frac{n(n+1)}{2}$ and its tangent space at each point is the vector space $\mathrm{Sym}(n)$. Let $A \in \mathrm{Sym}_+(n)$ and $K \in T_A \mathrm{Sym}_+(n) \cong \mathrm{Sym}(n)$. In this section we consider the Riemannian metric on the space

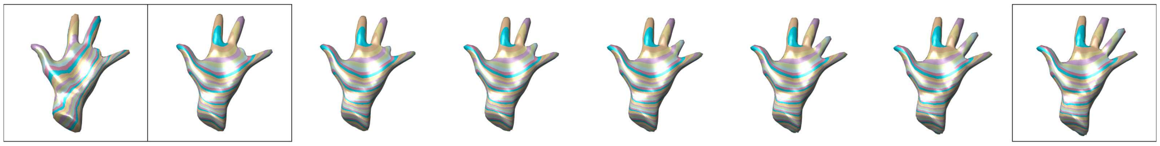

Figure 4. The matching and geodesic between two hand shapes in the space of unparametrized surfaces $\mathrm{Imm}(S^2, \mathbb{R}^3)/\mathrm{Diff}_+(S^2)$ with respect to the general elastic metric (1) for $a = 1, b = 1, c = 1$. The surface f_1 on the left and f_2 on the right show the original parametrizations of the boundary surfaces; the second one $f_1 \circ \gamma$ gives the final parametrization of the first boundary surface after the whole optimization process; the right 7 hand shapes show the interpolating geodesic between the two hand shapes. The geodesic is calculated with the method provided in [32] using the final point correspondence of our new algorithm.

$\mathrm{Sym}_+(n)$ induced by the DeWitt metric:

$$\langle K, K\rangle_A^\lambda = \mathrm{tr}(A^{-1}K_0A^{-1}K_0)\sqrt{\det(A)} + \lambda\left(\mathrm{tr}(A^{-1}K)\right)^2\sqrt{\det(A)}, \tag{9}$$

where $K_0 = K - \frac{1}{n}\mathrm{tr}(A^{-1}K)A$ is the traceless part of K. This Riemannian metric (9) is not affine invariant, but instead satisfies the following equivariance property, that is necessary for the reparametrization invariance of the DeWitt metric on the space of Riemannian metrics:

Theorem 5. *Let $A \in \mathrm{Sym}_+(n)$ and $K \in T_A\,\mathrm{Sym}_+(n)$. Then the family of metrics (9) is invariant under the following action of the group of invertible matrices:*

$$\mathrm{Sym}_+(n) \times \mathrm{GL}(n) \to \mathrm{Sym}_+(n)$$
$$(A, C) \mapsto C^T AC,$$

that is, given $C \in \mathrm{GL}(n)$ the following equality always holds:

$$\langle C^T KC, C^T KC\rangle_{C^TAC} = \langle K, K\rangle_A.$$

Proof. This result can be shown by direct calculation. □

For this family of metrics, the geodesic initial value problem on $\mathrm{Sym}_+(n)$ can be solved explicitly, see [15]:

Theorem 6. *Let $A \in \mathrm{Sym}_+(n)$ and $K \in T_A\,\mathrm{Sym}_+(n)$. Define*

$$r_1(t) = 1 + \frac{t}{4}\mathrm{tr}(A^{-1}K),$$
$$r_2(t) = \frac{t}{4}\sqrt{\lambda^{-1}\mathrm{tr}\left(A^{-1}K_0A^{-1}K_0\right)}.$$

If $K_0 \neq 0$, then the geodesic for the metric (9) in $\mathrm{Sym}_+(n)$ starting at A in the direction of K is given by

$$A_t = \left(r_1^2 + r_2^2\right)^{\frac{2}{n}} A \exp\left(\frac{t\arctan(r_2/r_1)}{r_2}A^{-1}K_0\right);$$

otherwise, if $K_0 = 0$, then the geodesic starting at A in the direction of K is given by $A_t = r_1^{\frac{4}{n}}A$.

Notice that if $K_0 = 0$ and $\mathrm{tr}(A^{-1}K) < 0$, then the geodesic will leave the space $\mathrm{Sym}_+(n)$ at time $T = -\frac{4}{\mathrm{tr}(A^{-1}K)}$. Thus the space $\mathrm{Sym}_+(n)$ is not geodesically complete.

Denote by $\widetilde{\mathrm{Sym}}_+(n)$ the space of positive semi-definite $n \times n$ symmetric matrices. The metric completion of $\mathrm{Sym}_+(n)$ is then given by the quotient $\overline{\mathrm{Sym}}(n) = \widetilde{\mathrm{Sym}}_+(n)/\sim$, where $A \sim B$ if they both are degenerate. In the metric completion $\overline{\mathrm{Sym}}(n)$, the minimal geodesic between any two points always exists and is unique.

Theorem 7. *Let $A, B \in \overline{\mathrm{Sym}}(n)$. Then there exists a unique minimal path between A and B. If either A or B is $[0]$ (the equivalence class of the 0 matrix), the minimal path is the line between A and B. Otherwise let $K = A\log(A^{-1}B)$, then the minimal path is given by*

(1) the geodesic connecting A and B if

$$\mathrm{tr}\left(A^{-1}K_0A^{-1}K_0\right) < (4\pi)^2\lambda,$$

(2) the concatenation of the straight line segments from A to 0 and from 0 to B if

$$\mathrm{tr}\left(A^{-1}K_0A^{-1}K_0\right) \geq (4\pi)^2\lambda.$$

Furthermore, the squared distance on the metric completion is explicitly given by

$$d^\lambda_{\overline{\mathrm{Sym}}}(A, B)^2 = 16\lambda\left(s_1^2 - 2s_1s_2\cos\theta + s_2^2\right),$$

where

$$s_1 = \sqrt[4]{\det(A)}, \qquad s_2 = \sqrt[4]{\det(B)},$$
$$K = \begin{cases} A\log(A^{-1}B) \text{ if } A \text{ and } B \text{ are non-degenerate} \\ 0 \text{ else} \end{cases}$$
$$\theta = \min\left\{\pi, \sqrt{\lambda^{-1}\mathrm{tr}\left(A^{-1}K_0A^{-1}K_0\right)}/4\right\}.$$

Proof. For $\lambda = \frac{1}{n}$ the result was proven on [11]. The general case follows by using the results of [11] and combining it with the explicit formulas of [15]. This would however exceed the scope of this conference paper and we thus refer from presenting the full proof here. □

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