THE CONTINUOUS PROCRUSTES DISTANCE BETWEEN TWO SURFACES

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Abstract. The Procrustes distance is used to quantify the similarity or dissimilarity of (3-dimensional) shapes, and extensively used in biological morphometrics. Typically each (normalized) shape is represented by \( N \) landmark points, chosen to be homologous (i.e. corresponding to each other), as much as possible, and the Procrustes distance is then computed as \( \inf_R \sum_{j=1}^{N} \| R x_j - x'_j \|^2 \), where the minimization is over all Euclidean transformations, and the correspondences \( x_j \leftrightarrow x'_j \) are picked in an optimal way.

This (discrete) Procrustes distance is easy to compute but has drawbacks – representing a shape by only a finite number of points, which may fail to capture all the geometric aspects of interest; a need has been expressed for alternatives that are still computationally tractable. We propose in this paper the concept of continuous Procrustes distance, and prove that it provides a true metric for two-dimensional surfaces embedded in three dimensions. The continuous Procrustes distance leads to a hard optimization problem over the group of area-preserving diffeomorphisms. One of the core observations of our paper is that for small continuous Procrustes distances, the global optimum of the Procrustes distance can be uniformly approximated by a conformal map. This observation leads to an efficient algorithm to calculate approximations to this new distance.

1. Introduction

Procrustes distances are used to compare shapes and quantify their (dis)similarity. In several applications, such as geometric morphometrics [13], the shapes to be compared are continuous surfaces, on each of which homologous landmark points are selected, equal in number. The dissimilarity or distance between the surfaces \( S \) and \( S' \) is then computed as the Procrustes distance between their corresponding landmark sequences \( X = (x_i)_{i=1}^{L} \) and \( X' = (x'_i)_{i=1}^{L} \), which is defined as follows.

Definition 1.1. Given two finite sequences \( X = (x_i)_{i=1}^{n} \), \( X' = (x'_i)_{i=1}^{n} \) in \( \mathbb{R}^{d} \), of equal length, with centroids \( \bar{x}, \bar{x}' \), and centroid sizes \( S_X, S_{X'} \), respectively\(^1\) the classical Procrustes distance \( d_{P}(X,X') \) between \( X \) and \( X' \) is defined by

\[
(1.1) \quad d_{P}(X,X') = \inf_{R \in \mathcal{R}} \left( \sum_{i=1}^{n} \left\| \frac{R x_i}{S_X} - \frac{x'_i}{S_{X'}} \right\|^2 \right)^{1/2},
\]

where \( \mathcal{R} \) is the group of Euclidean transformations (reflections, rotations, and translations).

In some applications, it may be useful to consider weighted Procrustes distances, in which each label \( i \in \{1, \ldots, L\} \) can be given its own weight \( w_i \) in the computation of the centroids, the centroid sizes and the distance \( d_{P}(X,X') \); such weighting can be used to compensate, if desired, for possible imbalances in the distribution of the landmark points, when they occur more densely in some areas than in others. We shall assume in what follows that no such adjustment is needed, i.e., that the landmark points are considered (more or less) uniformly distributed. The normalization by the centroid size allows comparison of shapes irrespective of their scale. To achieve this without a normalization step, one would need to extend \( \mathcal{R} \) to the larger group of similarities, incorporating the (uniform) dilations as well. Note that other geometric extensive quantities could be used to normalize, with a very similar effect.

\(^1\) The centroid of \( X \) is given by \( \bar{x} = n^{-1} \sum_{i=1}^{n} x_i \); the centroid size by \( S_X = [n^{-1} \sum_{i=1}^{n} (x_i - \bar{x})^2]^{1/2} \).
The point sets $X$ and $X'$ are said to have the same shape if one can be obtained from the other by an appropriate combination of scaling, translating, rotating and (possibly) mirroring, i.e., if there exists $R \in \mathbb{R}$ and $\alpha \in \mathbb{R}$ such that $\alpha RX = X'$. (“Shapes” of finite sets of points can thus be considered as orbits of these point sets under the action of similarity operations.) It is not hard to check that the Procrustes distance $d_p(\cdot, \cdot)$ is a metric on shapes, in the sense that it satisfies, for all finite point sequences $X$, $X'$ and $X''$ in $\mathbb{R}^d$ of equal length,

1) $d_p(X, X') = d_p(X', X)$,

2) $d_p(X, X') \geq 0$, and $d_p(X, X') = 0$ implies that $X$ and $X'$ have the same shape,

3) $d_p(X, X'') \leq d_p(X, X') + d_p(X', X'')$.

In all the above, the points $x_i$ and $x_i'$ are ordered, i.e. corresponding points in $X$ and $X'$ have the same index. The correspondence between entries of $X$ and $X'$ can be “encoded” by a bijective correspondence map $C : X \rightarrow X'$ that maps each $x_j \in X$ to its corresponding $x'_j \in X'$. In terms of this correspondence map the Procrustes distance $d_p(X, X')$ can be written as

$$d_p(X, X') = d_p(X, CX) = \inf_{R \in \mathbb{R}} \| RX - CX \| := \inf_{R \in \mathbb{R}} \left( \sum_{i=1}^n \| Rx_i - Cx_i \|^2 \right)^{1/2};$$

this recasts the minimization as a search for the map in $\mathbb{R}$ that best approximates $C$, insofar as its action on $X$ is concerned.

Using a finite set $X$ of landmark points $x_\ell \in S$, $\ell = 1, \ldots, L$ as a proxy for the shape of a surface $S$, and taking the value of $d_p(X, X')$ to express the dissimilarity of the shapes of surfaces $S$ and $S'$ has some drawbacks, however. First, this approach compares only small discrete subsets of points sampled from the surfaces and therefore ignores “most” of their shapes. Second, and more importantly, it requires the user to carefully select corresponding landmark points on the two surfaces prior to calculating the Procrustes distance between the two landmark point sequences. This distance depends heavily on the exact choice of the landmark points. In geometric morphometrics, one seeks to remove some of the arbitrariness of these choices by picking landmark points that are believed to be homologous, i.e., to truly correspond to each other, based on evolutionary arguments. This type of selection of landmark points requires considerable specialized expertise, and in some cases, even experts do not agree. In addition, morphologists interested in studying function of e.g. teeth are interested in moving away from landmark selection, and in using geometric information that encompasses more global features.

This situation has motivated researchers to suggest alternative methods to compute distances or dissimilarities between the shapes of surfaces. Even when these methods are based on continuous concepts, their numerical implementation requires some type of discretization, and thus often involves again discrete point sets $X$ and $X'$ (typically of larger cardinality than in landmark-based distances). The resulting distance can then still be written in the same form as the right hand side of 1.2, with the important difference that $C$ is no longer assumed to be given a priori. Instead, the map $C$ is assumed to be determined by the full geometry of the surfaces $S$ and $S'$; in practice, it has to be derived from the data themselves, meaning that both the correspondence $C$ and the Euclidean transformation $R$ must be determined numerically. (One could imagine a similar situation in the discrete case, if two sets $X$ and $X'$ were given, each with $n$ points, without a correspondence map. In that case, a reasonable approach might be to select the map $C : X \rightarrow X'$ for which $\| CX - X' \|$ is smallest.)

A prominent method of this type is the Iterative Closest Point (ICP) algorithm [3]. This method alternates between determining $C$ and $R$: the correspondence $C_k : X \rightarrow X'$ is taken to associate to each point $x' \in X'$ the point(s) in $X$ for which the image $R_{k-1}x$, under the best rigid alignment of $X$ and $X'$ obtained in the previous iteration, is closer to $x'$ than to any other element in $X'$; the rigid alignment $R_k$ is then the transformation $R \in \mathbb{R}$ that minimizes the distance $\|RX - C_k X\|$. This algorithm is simple and robust, but suffers from several drawbacks. It may converge to a local minimum rather than the desired minimizer; this means that the limit may depend on the choice of the initial correspondence map $C_1$ or the initial rigid alignment $R_0$, whichever is picked to start off the algorithm. Of more concern is that the space of possible
correspondences \( C : S \to S' \) considered by the algorithm consists only of compositions of rigid motions and closest neighbor maps. This space of maps often contains high-distortion and discontinuous mappings, as illustrated in Figure 1 for the 1-dimensional situation; it also does not include a sufficiently rich set of diffeomorphisms (smooth bijective mappings).

(a) The correspondence map \( C_1 : X \to X' \), in this case a length-preserving diffeomorphism. \( (S \) and \( S' \) each consist of 200 points, equispaced on the black horizontal line \( (X) \) and on the blue curve \( (X') \), respectively.)

(b) Illustration of the Euclidean map \( R_1 \) (moving the black line “up”) and the correspondence map \( C_2 \).

**Figure 1.** One-dimensional illustration of one step in the ICP algorithm. \( X \) and \( X' \) are point sets, each with 200 points, on two curves (“one-dimensional surfaces”) \( S \) (straight, black) and \( S' \) (wiggly, blue) of equal length. (a) The correspondence (in red) between \( X \) and \( X' \) that associates to each point \( x' \in X' \) the point \( x \in X \) at the same arclength distance from the left end point of its curve. (b) Using this correspondence as an initial \( C_1 : X \to X' \), determine the Euclidean transformation (now a simple translation in the plane) \( R_1 \) that minimizes \( \|R X - C_1 X\| \), and move \( X \) to \( R_1 X \); the red lines now link each \( R_1 x \in R_1 X \) to the closest point in \( X' \). The corresponding map \( C_2 : X \to X' \) is discontinuous and highly distorting.

Several authors have built extensions or generalizations of this approach, retaining the basic iterative principle of ICP, interleaving the determination of correspondences \( C_k \) and transformations \( R_k \) in successive steps. Rangarajan et al. [15] formulate a variant on the Procrustes distance between two discrete sets of points in which the correspondence maps are unknown \textit{a priori}. Their algorithm alternates between calculating optimal rotations and determining correspondence maps (bi-measures). For every fixed rotation \( R \), it computes the “measure coupling numbers” \( M_{ij} \) from one point set to another, minimizing the average of the squared residuals \( \sum_{i,j} M_{ij} \|R x_i - x'_j\| \), under the (soft) constraint that \( (M_{ij})_{i,j=1,...,n} \) is indeed a measure coupling. As is the case with ICP, this algorithm can still converge to a local rather than a global minimum, and the correspondence maps can still be “discontinuous and/or distorting”. Ghosh et al. [8] use a similar framework (although not related to Procrustes or any other distance) with a smooth surface deformation mechanism together with closest point maps to determine both the correspondence maps and the transformations in an alternating iterative procedure. The algorithm in [8] requires user initialization (which may influence the outcome); the way correspondences are assigned can lead the deformation mechanism to ultimately produce a distorting and/or discontinuous map between the surfaces.
A common characteristic of the algorithms mentioned above, which often (in the limit or in intermediate stages) lead to discontinuous or distorting correspondence maps, is that the space they explore (implicitly or explicitly) to build correspondence maps is insufficiently rich in smooth bijections.

In this paper we generalize the discrete Procrustes distance to continuous surfaces; in this formulation we use only \textit{smooth} correspondence maps. Our construction leads to a non-linear functional over a huge and non-linear space of possible maps that we call the \textit{continuous Procrustes functional}. Direct optimization, over its huge domain, of this generalized Procrustes functional is not feasible; we suggest that for many cases of interest, a different optimization suffices, over a (relatively) much smaller (and manageable) subset of all possible maps, consisting of conformal mappings combined with specific area-preserving maps. One of the main results of our paper is a proof that the class of conformal maps \textit{uniformly} approximates the globally optimal correspondence map in the regime where the continuous Procrustes functional takes on small values. Note that our approach thus provides a glimpse of the global minimizer (for the case of small continuous Procrustes distance) of a functional for which it is not known, in general, how to approximate the global minimizer in polynomial time.

In addition to the theoretical constructions, we also provide an efficient algorithm, without user interaction, to construct (an approximation to) the continuous Procrustes distance and the optimal correspondence map between two surfaces, again in the case where this distance is small, i.e. where the surfaces are not too dissimilar. In practice, this algorithm performs very well, and is sufficiently fast to be used for the computation of pairwise distances for all pairs in reasonably large collections of surfaces ($\sim 100$); see [10], a first presentation of the main results of this paper at a workshop in June 2010, as well as [2], which uses the algorithm explained here in detail for three biological data-sets.

A similar combination (conformal mappings composed with area-preserving maps) is used in the recent paper by Dominitz and Tannenbaum [5], to construct good mappings from surfaces to a Euclidean spherical domain. The goal of [5] is different, however; rather than seeking to define a distance between surfaces, that can be used for shape alignment, [5] is concerned with building a low distortion map from a surface to Euclidean domain, the inverse of which can then be used as a good parameterization for the surface.

The paper is organized as follows. In section 2, we introduce our definition of the continuous Procrustes distance for homeomorphic 2-dimensional compact surfaces embedded in $\mathbb{R}^3$; it involves a minimization that is unfeasible in practice. In section 3, we show that we can construct approximations of this distance by minimizing over appropriate perturbations of conformal mappings, which is much more tractable. In section 4, we give the corresponding numerical algorithm and illustrate them with a concrete example.

2. The Surfaces Procrustes Distance.

Consider two homeomorphic compact 2-dimensional surfaces $S, S'$ embedded in $\mathbb{R}^3$, endowed with the standard metric induced from their embedding. Because the biological applications that motivated this work require comparing shapes irrespective of scale (see [19] and reference therein), we are interested in defining a scale-independent distance. We shall therefore assume that the two surfaces are normalized to have unit volume (area):

$$\int_S d\text{vol}_S = 1 = \int_{S'} d\text{vol}_{S'}.$$

In building “good” correspondence maps between the continuous surfaces, we will be guided by what represents a “good” correspondence between discrete (relatively small) sets of points that “represent” the surfaces when standard Procrustes distances are used.

As mentioned in the introduction, great care is typically taken in the choice of sample points on surfaces that will then be used to compare the shapes of these surfaces. Landmark points on e.g. teeth or other bones are chosen so that they are homologous, i.e. “equivalent” from an evolutionary point of view. We are aiming for a landmark-free method; information of this type will thus not be available. Instead, we can use only geometric information given by the surface itself. Note that in (1.1), the different points $z_i$ all play an equal role. When choosing discrete sets $X, X'$, each consisting of $n$ points, on the surfaces $S$ and $S'$ to represent
their respective “shapes”, with the purpose of using them in a Procrustes distance calculation (1.1), it seems therefore reasonable to pick the points so that each represents an equal “share” of the surfaces; we shall interpret this here as representing an equal portion of the area of the surfaces. A correspondence map $C$ that maps each $x_i$ to its partner $x_i'$ can thus be interpreted as mapping portions of area 1/n of $S$ to the corresponding portions of $S'$ that have equal area; on the other hand, the sum in (1.1) can be viewed (up to a normalization) as a Riemann sum approximation to the integral of $\|Rx - Cx\|$ over $S$.

This analysis suggests the following “continuous analogue” of the discrete construction. To involve the whole surface $S$ (instead of just a set of sample points), we take $C$ to be an area-preserving map from $S$ to $S'$; for each fixed area-preserving $C$, we then define

$$d_P(S, S'; C) = \inf_{R \in \mathcal{R}} \left( \int_S \|Rx - Cx\|^2 \, d\text{vol}_S(x) \right)^{1/2}.$$  \hspace{1cm} (2.1)

In the absence of landmark-type or other user-guided information we have to select $C$ based solely on geometric information. Taking our cue from the discrete case, we want, given points $(x_i)_{i=1,\ldots,n}$ on $S$, to determine $(x_i')_{i=1,\ldots,n}$ on $S'$ so that each $x_i'$ corresponds “as well as possible” to $x_i$. In other words, this suggests that $C$ be picked so that $S'$ and $CS$ are optimally aligned, and that the continuous Procrustes distance be given by the corresponding value of $d_P(S, S'; C)$. More explicitly, defining $\mathcal{A}(S, S')$ to be the set of diffeomorphisms (smooth bijective maps with a smooth inverse) from $S$ to $S'$ that are area-preserving, we set

$$\mathbf{D}_{C,P}(S, S') = \inf_{C \in \mathcal{A}(S, S')} \left[ \inf_{R \in \mathcal{R}} \left( \int_S \|Rx - Cx\|^2 \, d\text{vol}_S(x) \right)^{1/2} \right].$$  \hspace{1cm} (2.2)

In the remainder of this section, we establish several properties for the quantities defined in (2.1) and (2.2), establishing, among other results, that $\mathbf{D}_{C,P}(\cdot, \cdot)$ defines a metric distance.

We start by proving that the minimum in (2.1) is always attained.

**Proposition 2.1.** Given two homeomorphic surfaces $S$, $S'$ of unit area, and an area-preserving map $C$ from $S$ to $S'$, there exists a rigid motion $R^* \in \mathcal{R}$ minimizing the functional $\int_S \|Rx - Cx\|^2 \, d\text{vol}_S(x)$.

**Proof.** Let $R_n \in \mathcal{R}$ be a sequence such that

$$\left( \int_S \|R_n x - Cx\|^2 \, d\text{vol}_S(x) \right) - d_P(S, S'; C)^2 < \frac{1}{n}.$$

Let us represent each rigid motion as a composition of an orthogonal transformation and a translation:

$$R_n x = U_n x + t_n,$$

where $U_n \in \mathbb{R}^{3 \times 3}$ and $t_n \in \mathbb{R}^3$. Thinking of $R_n = (U_n, t_n)$ as a vector in $\mathbb{R}^{12}$ it is clear that there exists some compact set $A \subset \mathbb{R}^{12}$ such that $R_n \in A$ for all $n$. Indeed, the orthogonal group $O(3)$ in its representation as a $3 \times 3$ matrix group is a compact set, and for sufficiently large $n$, the $t_n$ will all lie within some ball, i.e. $|t_n| < M$ for some $M$. Hence there exists some rigid transformation $R^* = (U^*, t^*)$ such that, up to extracting a subsequence, $R_n \to R^*$ as $n \to \infty$. Lastly, $R^*$ realizes the infimum $d_P(S, S'; C)$ since $\|U_n x + t_n - Cx\| \to \|U^* x + t^* - Cx\|$ for every $x \in S$, and similar arguments as above imply that $\|U_n x + t_n - Cx\|$ is bounded uniformly in $n$ and $x \in S$. The result then follows from the dominated convergence theorem. \Halmos

The following two propositions provide closed form solutions for (2.1); their proofs follow the discrete case in a rather straightforward manner. Note that we use that $C$ is area-preserving to establish these formulas (for the translation part). First, we show that the translational part $t^*$ takes the centroid of $S$ to the centroid of $S'$:

**Proposition 2.2.** If $S$ and $S'$ both have their centroids at the origin, i.e. $\int_S x \, d\text{vol}_S(x) = 0 = \int_{S'} y \, d\text{vol}_{S'}(y)$, then the translational part $t^*$ of the optimal rigid motion $R^*$ is zero.
Proof. Assume the surfaces $S$, $S'$ are centered as described in the assumptions of the theorem. Differentiating $\int_S \|Ux - Cx\|^2 \, d\text{vol}_S(x)$ with respect to each of the coordinates of the vector $t$ and plugging in $U = U^*$ and $t = t^*$, we get

$$0 = 2 \int_S (U^* x + t^* - Cx) \, d\text{vol}_S(x).$$

Rearranging the above equality and remembering that $S$ and $S'$ have unit area, we get

$$t^* = \int_S Cx \, d\text{vol}_S(x) - \int_S U^* x \, d\text{vol}_S(x)$$

$$= \int_{S'} y \, d\text{vol}_{S'}(y) - U^* \int_S x \, d\text{vol}_S(x) = 0.$$

\[\square\]

Next, the orthogonal transformation part:

**Proposition 2.3.** If $S$ and $S'$ both have their centroids at the origin, i.e. $\int_S x \, d\text{vol}_S(x) = 0 = \int_{S'} y \, d\text{vol}_{S'}(y)$, then the optimal orthogonal transformation $U^*$ can be written as

$$U^* = WQ^T,$$

where $W, Q$ are the orthogonal transformations from the Singular Value Decomposition (SVD)

$$\int_S x (Cx)^T \, d\text{vol}_S(x) = QSW^T,$$

where $S = \text{diag}(\sigma_1, \sigma_2, \sigma_3)$ is a diagonal matrix with the singular values of $U^*$ on the diagonal.

Proof. Expanding $\int_S \|Ux - Cx\|^2 \, d\text{vol}_S(x)$ we get:

$$\int_S \|Ux - Cx\|^2 \, d\text{vol}_S(x) =$$

$$\int_S \|x\|^2 \, d\text{vol}_S(x) - 2 \int_S x^T U^T Cx \, d\text{vol}_S(x) + \int_S \|Cx\|^2 \, d\text{vol}_S(x),$$

where we used that $U^T U = Id$. The sought-for $U^*$ therefore must maximize

$$E(U) = \int_S x^T U^T Cx \, d\text{vol}_S(x).$$

Note that

$$x^T U^T Cx = tr \left( x^T U^T Cx \right) = tr \left( Ux (Cx)^T \right),$$

and therefore

$$E(U) = tr \left[ U \int_S x (Cx)^T \, d\text{vol}_S(x) \right] = tr \left[ UQSW^T \right]$$

$$= tr \left[ W^T UQS \right] = tr \left[ \tilde{U} S \right] = \tilde{U}_{1,1} \sigma_1 + \tilde{U}_{2,2} \sigma_2 + \tilde{U}_{3,3} \sigma_3,$$

where $\tilde{U} := W^T UQ$, and we used the SVD decomposition. Note that the last term cannot be greater than $\sigma_1 + \sigma_2 + \sigma_3$ since all entries of the orthogonal matrix $\tilde{U}$ have absolute value at most 1. Further note that taking $U = WQ^T$ achieves this upper bound. The uniqueness is also clear. \[\square\]

We now prove:

**Proposition 2.4.** For each fixed area-preserving map $C$ from $S$ to $S'$, we have

1. $d_P(S, S'; C) \geq 0$
2. $d_P(S, S'; C) = d_P(S', S; C^{-1})$
3. $d_P(S, S'; C) = 0$ implies that $S$ and $S'$ are congruent.
Moreover, if $S''$ is a third surface, and $C'$ is an area-preserving map from $S'$ to $S''$, then

$$d_P(S, S''; C' \circ C) \leq d_P(S, S'; C) + d_P(S', S''; C').$$

Proof. First, it is clear that $d_P(S, S'; C) \geq 0$. If $d_P(S, S'; C) = 0$, then we know by Proposition 2.1 that there exists a rigid transformation $R^*$ such that

$$\int_S \|R^*x - Cx\|^2 d\text{vol}_S(x) = 0.$$

Since we are dealing with smooth surfaces $S$, this implies that $\|R^*x - Cx\| = 0$ for all $x \in S$; since the range of $C$ is all of $S'$ (because $C$ is a bijective diffeomorphism) it follows that $R^*S$ and $S'$ are equal as sets, so $S$ and $S'$ are congruent.

Next we prove symmetry:

$$d_P(S, S'; C)^2 = \inf_{R \in \mathcal{R}} \left( \int_S \|Rx - Cx\|^2 d\text{vol}_S(x) \right)^{1/2} = \inf_{R \in \mathcal{R}} \left( \int_{S'} \|R^{-1}y - y\|^2 d\text{vol}_{S'}(y) \right)^{1/2},$$

where the second equality uses the fact that $C$ is area-preserving.

For arbitrary $\tilde{R} \in \mathcal{R}$, we have

$$d_P(S, S''; C' \circ C) = \inf_{R \in \mathcal{R}} \left( \int_S \|Rx - C' \circ Cx\|^2 d\text{vol}_S(x) \right)^{1/2} \leq \inf_{R \in \mathcal{R}} \left( \int_S \|Rx - \tilde{R}Cx\|^2 d\text{vol}_S(x) \right)^{1/2} + \int_S \|\tilde{R}C - C' \circ C\|^2 d\text{vol}_S(x)^{1/2} = \inf_{R \in \mathcal{R}} \left( \int_S \|Rx - Cx\|^2 d\text{vol}_S(x) \right)^{1/2} + \int_{S'} \|\tilde{R}y - C'y\|^2 d\text{vol}_{S'}(y) \right)^{1/2},$$

By taking the infimum over all $\tilde{R} \in \mathcal{R}$ we obtain the desired result.

Having established these properties for $d_P(S, S'; C)$, we can now minimize this over $C \in \mathcal{A}(S, S')$, i.e. we have

$$(2.3) \quad D_{cP}(S, S') = \inf_{C \in \mathcal{A}(S, S')} d_P(S, S'; C);$$

if the infimum is achieved by some $C^* \in \mathcal{C}$, we declare this $C^*$ to be our desired correspondence map.

Whether such a minimizer exists is a delicate question, and we do not have a proof or counter example for the general case. However, if we restrict the class of maps $C$ to bi-Lipschitz maps with some a priori bound on the maximal dilation, then such a minimizer does indeed exist; moreover this minimizer is also bi-Lipschitz with the same bound.

**Proposition 2.5.** For arbitrary $B > 0$, let $\mathcal{B}_B(S, S')$ be the set of bi-Lipschitz area-preserving diffeomorphisms from $S$ to $S'$ such that, for all $x, y \in S$, $B^{-1}d_S(x, y) \leq d_{S'}(Cx, Cy) \leq Bd_S(x, y)$, and let $d_S$, resp. $d_{S'}$ denote the geodesic distances on $S$, resp. $S'$. Then there exists a minimizer in $\mathcal{B}_B(S, S')$ for the restriction to $\mathcal{B}_B(S, S')$ of the functional $D_{cP}(S, S'; \cdot)$.

Proof. It is straightforward that $\mathcal{B}_B(S, S')$ is a closed subset of $C(S, S')$, the set of continuous functions from $S$ to $S'$, equipped with the topology of uniform convergence with respect to $d_S$ and $d_{S'}$. By the definition of $\mathcal{B}_B(S, S')$, the functions in $\mathcal{B}_B$ are equicontinuous. It then follows from the Ascoli-Arzelà theorem for the
continuous functions on compact metric spaces that $B_B(S, S')$ is compact.
It is also easy to see that the functional $d_P(S, S'; \cdot)$ is continuous with respect to the topology of uniform convergence on $C(S, S')$. It follows that the restriction of $d_P(S, S'; \cdot)$ to $B_B(S, S')$ is a continuous map from a compact space to $\mathbb{R}$. Let now $(C_n)_{n \in \mathbb{N}}$ be a minimizing sequence in $B_B(S, S')$, i.e. $d_P(S, S'; C_n) \to \inf_{C \in B_B(S, S')} d_P(S, S'; C)$ as $n \to \infty$. By the compactness of $B_B(S, S')$, the sequence $(C_n)_{n \in \mathbb{N}}$ has a uniformly converging subsequence; if we denote its limit by $C^*$, then it follows that $C^* \in B_B(S, S')$, and $d_P(S, S'; C^*) = \inf_{C \in B_B(S, S')} d_P(S, S'; C)$. \hfill $\square$

We note here that all the further proofs and results in the paper will remain valid (mutatis mutandum) if we replace everywhere the class of general area-preserving maps by the more restricted class of bi-Lipschitz area-preserving maps.

Even when the existence of a minimizer is not guaranteed, it is possible to prove that $D_c(P(S, S'))$ defines a metric up-to congruence relation:

**Theorem 2.6.** $D_c(P(S, S'))$ defines a metric between surfaces up-to congruence, that is, $D_c(P(S, S')) \geq 0$, $D_c(P(S, S')) = D_c(P(S', S))$, $D_c(P(S, S')) \leq D_c(P(S, S'') + D_c(P(S'', S'))$, and $D_c(P(S, S')) = 0$ only if $S$ and $S'$ are congruent.

**Proof.** Clearly $D_c(P(S, S')) \geq 0$.

If $D_c(P(S, S')) = 0$ then we have a sequence $(C_n)_{n \in \mathbb{N}} \subset A(S, S')$ and (by Proposition 2.1) a sequence $(\tilde{R}_n)_{n \in \mathbb{N}} \subset \mathcal{R}$ of rigid motions such that:

$$\int_S \|R_n x - C_n x\|^2 d\nu_S(x) < \frac{1}{n^3}.$$ 

By extracting a subsequence $(\tilde{R}_{n_k}^*)_{k \in \mathbb{N}}$ (with $\tilde{R}_{n_k}^* := \tilde{R}_{n_k}$), we can assume that $\|R_{n_k}^* - R^{**}\|_\infty \to 0$, with $R^{**} \in \mathcal{R}$ as $k \to \infty$, and that (with $C_{n_k}^* := C_{n_k}$)

$$\int_S \|R^{**} x - C_{n_k}^* x\|^2 d\nu_S(x) < \frac{1}{k^3}.$$ 

Set now $B_{n, \ell} := \{x; \|R^{**} x - C_{n_k}^* x\|^2 \geq 1/\ell\}$, $A_{\ell} := \{x; \limsup_{k \to \infty} \|R^{**} x - C_{n_k}^* x\|^2 \geq 1/\ell\} = \bigcap_{m \in \mathbb{N}} \bigcup_{n \geq m} B_{n, \ell}$, and $A_{\infty} := \bigcup_{\ell \geq 1} A_{\ell} = \{x; \limsup_{k \to \infty} \|R^{**} x - C_{n_k}^* x\|^2 \neq 0\}$. Since $A_\ell \subset A_{\ell+1}$ for all $\ell$, it follows that $\lim_{\ell \to \infty} \nu_S(A_\ell) = \nu_S(A_\infty) = 0$. We have $\lim_{\ell \to \infty} \|R^{**} x - C_{n_k}^* x\|^2 d\nu_S(x) \leq \|R^{**} x - C_{n_k}^* x\|^2 d\nu_S(x) \leq \frac{1}{k^3}$, hence $\lim_{\ell \to \infty} \|R^{**} x - C_{n_k}^* x\|^2 d\nu_S(x) \leq \frac{1}{k^3}$.

Therefore $R^{**} x = \lim_{k \to \infty} C_{n_k}(x)$ for $x \in S \setminus A_\infty$, implying $R^{**}(S \setminus A_\infty) \subset S'$. Since every open disk in $S$ (with respect to the geodesic distance on $S$) has area strictly greater than 0 in $S$, $S \setminus A_\infty$ is dense in $S$. By the continuity of $R^{**}$ it follows that $R^{**}(S) \subset S'$.

Let’s assume now (hoping to derive a contradiction) that there exists a point $\tilde{y} \in S'$ such that $\tilde{y} \notin R^{**}(S)$. Since $R^{**}(S)$ is a closed set there must then exist a set $O \subset S'$ with positive area such that $O \cap R^{**}(S) = \emptyset$. This is a contradiction since $R^{**}: S \to S'$ is an isometry and in particular area-preserving. Hence $R^{**}(S) = S'$, showing that $S$ and $S'$ are congruent.

Symmetry is easy to establish as follows:

$$D_c(P(S, S')) = \inf_{C \in A(S, S')} d_P(S, S'; C) = \inf_{C \in A(S, S')} d_P(S', S; C^{-1})$$

$$= \inf_{C \in A(S', S)} d_P(S', S; C) = D_c(P(S', S)),$$

where we used that $C \in A(S, S')$ iff $C^{-1} \in A(S', S)$. 

Lastly, for the triangle inequality, we have, by Theorem 2.4 for every \( C \in \mathcal{A}(S, S') \) and every \( C' \in \mathcal{A}(S', S'') \),
\[
D_{cP}(S, S'') = \inf_{C'' \in \mathcal{A}(S, S'')} d_P(S, S''; C'') \leq d_P(S, S''; C) \leq d_P(S, S'; C) + d_P(S', S''; C').
\]

Taking the infimum over \( C \in \mathcal{A}(S, S') \) and \( C' \in \mathcal{A}(S', S'') \) we get
\[
D_{cP}(S, S'') \leq \inf_{C \in \mathcal{A}(S, S')} d_P(S, S'; C) + \inf_{C' \in \mathcal{A}(S', S'')} d_P(S', S''; C') = D_{cP}(S, S') + D_{cP}(S', S'').
\]

We conclude this section by providing an approximation result: given two surfaces \( S \) and \( S' \) and a correspondence map \( C \in \mathcal{A}(S, S') \), we would like to approximate the centroids \( \mathbb{E}(S) \) and \( \mathbb{E}(S') \) without including any point of the (discrete) set \( C \). Using the notation \( \text{vol}(S) = \int_S \, dvol_S(x) \) and \( \text{vol}(C) = \sum_{x \in C} \text{vol}(S_x) \) we then have
\[
(2.4) \quad \int_S f(x) dvol_S(x) \approx \sum_{\ell} f(q_\ell) \text{vol}(S_\ell).
\]

The error made in this approximation can be estimated in terms of the fill distance \( \eta(S, Q) \) of the set \( Q \), defined as
\[
(2.5) \quad \eta(S, Q) := \sup \left\{ r \in \mathbb{R} \mid \exists x \in M \text{ s.t. } B_S(x, r) \cap Q = \emptyset \right\},
\]
where \( B_S(x, r) = \{ q \in S \mid d_S(x, q) < r \} \), with \( d_S(x, q) \) the geodesic distance on \( S \) between \( x \) and \( q \). Intuitively, the fill distance \( \eta(S, Q) \) is the radius of the largest geodesic open ball that can be placed on the surface \( S \) without including any point of the (discrete) set \( Q \). In other words it is the largest “circular hole” in the sampling \( Q \subset S \). We have then

**Proposition 2.7.** The error of the approximation \( (2.4) \) has the following upper bound:
\[
\left| \int_S f(x) dvol_S(x) - \sum_{\ell} f(q_\ell) \text{vol}(S_\ell) \right| \leq \sup_{\ell, x \in S_\ell} |f(x) - f(q_\ell)| \leq M \eta(S, Q),
\]
where \( M \) is a bound on the norm of the gradient \( \nabla_S f \) of \( f \). Hence the error is linear in the separation distance.

**Proof.** Writing \( S = \bigcup_{\ell} S_\ell \) we get
\[
\left| \int_S f(x) dvol_S(x) - \sum_{\ell} f(q_\ell) \text{vol}(S_\ell) \right| \leq \sum_{\ell} \int_{S_\ell} |f(x) - f(q_\ell)| dvol_S(x) \leq \sup_{\ell, x \in S_\ell} |f(x) - f(q_\ell)| \sum_{\ell} \text{vol}(S_\ell) = \sup_{\ell, x \in S_\ell} |f(x) - f(q_\ell)|,
\]
where the last equality uses \( \text{vol}(S) = 1 \). Now take arbitrary \( x \in S_\ell \), and denote by \( \gamma(t) : [0, d_S(q_\ell, x)] \rightarrow S \) the arc-length speed geodesic curve connecting \( q_\ell \) and \( x \). Then,
\[
f(x) - f(q_\ell) = \int_0^{d_S(q_\ell, x)} \frac{d}{dt} [f(\gamma(t))] dt = \int_0^{d_S(q_\ell, x)} \langle \nabla_S f(\gamma(t)), \dot{\gamma}(t) \rangle_S dt.
\]
Using the Cauchy-Schwarz inequality,

$$|f(x) - f(q_t)| \leq \sup_{x \in S} \|\nabla_S f(x)\|_S \int_0^{d_S(q_t,x)} \|\dot{\gamma}(t)\|_S dt = \sup_{x \in S} \|\nabla_S f(x)\|_S d_S(q_t,x).$$

Lastly, the inequality $d_S(q_t,x) \leq \eta(S)$ can be derived directly from the properties of Voronoi cells (see Lemma D.2 in [12]).

### 3. Möbius transformations as a reduced search space

Computing the surface Procrustes distance, as we defined it above, amounts to solving a hard optimization problem: unfortunately, the sets $A(S,S')$ or $B_B(S,S')$ are formally infinite dimensional manifolds, and therefore extremely hard to search in practice. Our key idea is to replace the search space $A(S,S')$ in the variational formulation (2.3) by another, much smaller, set of maps. The core observation is that the set of conformal (or anti-conformal) mappings between $S$ and $S'$, which has a finite (and small) dimensionality, gets “close” (in some sense to be made precise below) to the minimizing $C \in A(S,S')$. In particular, we shall see that if $D_{\text{Pr}}(S,S')$ is small, then the minimizing area-preserving map $C$ in (2.3) is close to conformal.

Let us explain this in some more detail. We are particularly interested in computing (approximate) continuous Procrustes distances for “close” pairs [4]. In those cases the insight that (close to) optimal $C$ have to be close to conformal leads us to a strategy that involves minimizing over a much smaller set of maps. To achieve this, we shall make use of a nonlinear procedure $Pr$ that “transforms” a map that is close to $A(S,S')$ into an area-preserving map, i.e. to an element of $A(S,S')$. This nonlinear transformation leaves elements of $A(S,S')$ unchanged, and can thus be interpreted as a nonlinear projection procedure (hence the notation). The smaller set of maps over which we shall minimize is then the image in $A(S,S')$ of the family of conformal maps (from $S$ to $S'$), transformed by $Pr$.

As a search space, the family of conformal mappings is a much more “friendly” setting than $A(S,S')$ or $B_B(S,S')$. First, by the uniformization theorem the conformal (or anti-conformal) bijective mappings can be characterized completely, and an explicit parameterization can be given in terms of a small number of parameters. For instance, the family of conformal bijective mappings between two disk-type surfaces $S, S'$ is represented by (disk-preserving) Möbius transformations. Each mapping in this family is completely characterized by 3 real (bounded) parameters; therefore the search over the space of conformal mappings can be done efficiently. Second, Möbius transformations are smooth bijective diffeomorphisms, so that our candidate search space consists of only “nice” intrinsic mappings.

To motivate why we would consider restricting ourselves to conformal mappings (or their deformations through $Pr$) for the optimization, we note that for $S, S'$ such that $D_{\text{Pr}}(S,S') = 0$, the infimum in (2.3) is achieved for some $R \in R$ (by Theorem 2.4); in this case the minimizing $C = R$ is obviously conformal. However, we prove below the stronger result that a correspondence $C : S \rightarrow S'$ for which the distance $d_P(S,S';C)$ is small can be approximated (under rather mild assumptions on the regularity of $C$) by a bijective globally conformal mapping from $S$ to $S'$.

We start with a few simple lemmas. The first Lemma is proved in [10];

**Lemma 3.1.** Let $S \subset \mathbb{R}^3$ be a compact 2-manifold with the induced Riemannian metric $g$. Then

$$|d_S(x,x') - \|x-x'\| | \leq C_S d_S(x,x')^3,$$

where $d_S(x,x')$ denotes the geodesic distance between $x$ and $x'$, $\|x-x'\|$ denotes the Euclidean distance between these points, and $C_S$ depends only on the curvature of $S$.

Next, we prove a result concerning the approximation of the norm of the differential of a map:
Lemma 3.2. Let $S, S' \subset \mathbb{R}^3$ be compact 2-manifolds with the induced Riemannian metrics $g, h$ (respectively). Let $F : S \to S'$ be a smooth map, and denote by $DF_x$ the differential of $F$ at arbitrary $x \in S$. Then for $\delta > 0$ sufficiently small, the following holds: for all $x \in S$, there exists $x'$ in the boundary $\partial B_g(x, \delta)$ of the $\delta$-radius geodesic ball centered at $x$, $\partial B_g(x, \delta) := \{ u \in S | d_S(x, u) = \delta \}$, such that

$$\frac{\|F(x) - F(x')\|}{\|x - x'\|} - \|DF_x\|_{g,h} \leq C_\kappa \delta,$$

where $\|\|_{g,h}$ is the operator norm associated with the norms $\|\|_g$ and $\|\|_h$ in the usual way, i.e. $\|L\|_{g,h} = \sup_{\xi \neq 0} \frac{\|L\xi\|_h}{\|\xi\|_g}$. Here, $C_\kappa$ depends only on the maximum of the surfaces’ curvature and norms of second order differentials of the mapping $F$.

Proof. For $\xi \in \mathbb{R}^2$, we set $D(\delta) = \{ \xi \in \mathbb{R}^2 | \|\xi\| \leq \delta \}$. Fix $x$ and take $\delta > 0$ small enough so that the exponential map $exp_x : D(2\delta) \to B_g(x, 2\delta)$ is a diffeomorphism. For every $x' \in B_g(x, \delta)$, we denote by the vector $\xi_{x'}$ the vector in $D(\delta)$ such that $exp_x(\xi_{x'}) = x'$; in other words, $\xi_{x'}$ is tangent to the geodesic on $S$ that goes from $x$ to $x'$, and $\|\xi_{x'}\| = d_S(x, x')$. Denote $\tilde{F} = F \circ exp_x : D(\delta) \to S'$, and consider the line $\gamma(t) = t \xi_{x'}$, $0 \leq t \leq 1$. Then

$$F(x') - F(x) = \int_0^1 \frac{d}{dt} [\tilde{F}(\gamma(t))] dt = \int_0^1 D\tilde{F}_{\gamma(t)} \dot{\gamma}(t) dt = \int_0^1 \left( D\tilde{F}_{\gamma(t)} + O(\|\xi_{x'}\|) \right) \xi_{x'} dt = D\tilde{F}_{x'} + O(d_S(x, x')^2).$$

(3.1)

Let $\xi \in \partial D(\delta)$ be such that $\|D\tilde{F}_{x}(\xi)\|_h = \|D\tilde{F}_{x}\|_{g,h} \|\xi\|_g$. Remember that at $exp^{-1}(x)$ the pull-back metric tensor $(exp^*_x g)$ equals $\delta_{ij}$, and therefore $\|\xi\|_g = \|\xi\|$. Also note that $\|D\tilde{F}_{x}(\xi)\|_h = \|D\tilde{F}_{x}(\xi)\|$, since the metric $h$ is induced by the ambient Euclidean metric of $\mathbb{R}^3$. Now set $x' = exp_x(\xi)$, and take the Euclidean norm of both sides of (3.1). Then we have

$$\|F(x') - F(x)\| = \|D\tilde{F}_{x}\|_{g,h} d_S(x, x') + O(d_S(x, x')^2),$$

and therefore

$$\frac{\|F(x') - F(x)\|}{d_S(x, x')} = \|D\tilde{F}_{x}\|_{g,h} + O(d_S(x, x')).$$

Using Lemma 3.1, this leads to the desired estimate. \hfill \Box

Next, we define the cone condition for a surface $S$:

**Definition 3.3.** We say that a compact 2-manifold $S \subset \mathbb{R}^3$ satisfies the $(\sigma, \theta)$-cone condition, where $\sigma > 0$ and $\theta \in (0, 2\pi)$, if for every $x \in S$ there is a unit vector $n$ in the tangent plane $T_x S$ such that the exponential map $exp_x$ is well-defined on the cone $c_S(\sigma, \theta; n) = \{ \xi \in \mathbb{R}^2 | \|\xi\| \leq \sigma, \langle \xi, n \rangle \geq \|\xi\| \cos(\theta/2) \}$, and is one-to-one on the whole cone.

In other words, the surface $S$ satisfies the $(\sigma, \theta)$-cone condition if for every $x \in S$, there is a “fan”, spanning at least an angle $\theta$, of geodesics that leave $x$ and continue, within $S$, for at least a distance $\sigma$ (w.r.t. the metric induced on $S$ by $\mathbb{R}^3$), without intersecting themselves or any other geodesic in the fan. We have now

**Lemma 3.4.** Let $S \subset \mathbb{R}^3$ be a compact 2-manifold satisfying the $(\sigma, \theta)$-cone condition. Then there exist constants $\rho, \Gamma > 0$ depending on $\sigma, \theta$ and on the curvature $\kappa$ of $S$ such that for all $u \in S$ and all $r < \rho$, the area of $\{ x \in S | \|u - x\| \leq r \}$ is bounded below by $\Gamma r^2$ (with $\|\|$ standing for the Euclidean norm in $\mathbb{R}^3$).
Proof. By Lemma 3.1 there exists a constant \( R > 0 \) (depending only on the curvature of \( \mathcal{S} \)) such that for all \( x, y \in \mathcal{S} \) satisfying \( d_{\mathcal{S}}(x, y) < R \) we have \[ d_{\mathcal{S}}(x, y) > \frac{1}{2} \| x - y \| . \]

Set \( \rho_0 = 2 \min \{ R, \sigma \} \), and fix an arbitrary \( u \in \mathcal{S} \). We have then, for all \( r < \rho_0 \), that \( \{ x \in \mathcal{S} \mid d_{\mathcal{S}}(u, x) \leq r/2 \} \subset \{ x \in \mathcal{S} \mid \| u - x \| \leq r \} \), and consequently

\[
\int_{\{ x \in \mathcal{S} \mid \| u - x \| \leq r \}} d\text{vol}_{\mathcal{S}}(x) \geq \int_{\{ x \in \mathcal{S} \mid d_{\mathcal{S}}(u, x) \leq r/2 \}} d\text{vol}_{\mathcal{S}}(x).
\]

Now introduce polar coordinates \((\tau, \phi)\) on the tangent plane \( T_u \mathcal{S} \), so that the vector \( n \) (with respect to which the cone condition holds at \( u \)) is aligned with the direction \( \phi = 0 \). With respect to this coordinate system, the exponential \( \exp_u \) maps \([0, \sigma] \times [-\theta/2, \theta/2] \) to \( \mathcal{S} \), and the metric density can be written as [17]:

\[
\sqrt{g(\tau, \phi)} = \tau - \tau^3 \frac{\kappa(u)}{6} + o(\tau^3).
\]

Since \( r < \rho_0 \leq 2\sigma \), the sector \([0, r/2] \times [-\theta/2, \theta/2] \) is contained in \([0, \sigma] \times [-\theta/2, \theta/2] \) and we have

\[
\int_{\{ x \in \mathcal{S} \mid d_{\mathcal{S}}(x, y) \leq r/2 \}} d\text{vol}_{\mathcal{S}}(x) \geq \int_{-\theta/2}^{\theta/2} \int_0^{r/2} \sqrt{g(\tau, \phi)} d\tau d\phi
\]

\[
= r^2 \theta - r^4 \frac{\kappa(u) \theta^3}{384} + o(r^4) = r^2 \theta \left( 1 + O(r^2) \right),
\]

where, as usual, the absolute value of the \( O(r^2) \) term is bounded above by \( Cr^2 \), for some \( C > 0 \), for all \( r \) smaller than some \( r_1 \). Setting \( \rho = \min(\rho_0, r_1, 1/\sqrt{2C}) \) and \( \Gamma = [1 - \min(1/2, C r^2)] \theta/8 \) we obtain, for \( r < \rho \),

\[
\int_{\{ x \in \mathcal{S} \mid d_{\mathcal{S}}(x, y) \leq r/2 \}} d\text{vol}_{\mathcal{S}}(x) \geq \Gamma r^2,
\]

completing the proof. \( \square \)

We are ready to prove the main result of this section, which provides a bound on the conformal distortion \( d_{\mathcal{S}} \) of the optimal area-preserving “alignments” \( C \) for surfaces \( \mathcal{S} \) and \( \mathcal{S}' \) that are close to each other in the continuous Procrustes distance. The conformal distortion \( d_{\mathcal{S}}(x) \) of \( \mathcal{C} \) at \( x \) is defined as the ratio between the two singular values of the matrix obtained by expressing the differential \( DC_x \) with respect to orthonormal bases in \( T_x \mathcal{S} \) and \( T_{C_x} \mathcal{S}' \), respectively.

**Theorem 3.5.** Let \( \mathcal{S}, \mathcal{S}' \subset \mathbb{R}^3 \) be 2-manifolds with induced Riemannian metrics \( g, h \) (respectively), with curvatures bounded above by \( \kappa \), and satisfying the \((\sigma, \theta)-cone\) condition. We consider area-preserving diffeomorphisms \( \mathcal{C} : \mathcal{S} \to \mathcal{S}' \) with first and second order differentials bounded by \( \mathcal{M} \). Then, for sufficiently small \( \epsilon \), the bound \( d_{\mathcal{P}}(\mathcal{S}, \mathcal{S}'; \mathcal{C}) \leq \epsilon \) implies the following bound on the conformal distortion \( d_{\mathcal{S}}(x) \) of the map \( \mathcal{C} \):

\[
\sup_{x \in \mathcal{S}} d_{\mathcal{S}}(x) \leq 1 + O(\epsilon^{1/4}),
\]

where the constant in the \( O \)-notation depends only on \( \kappa \) and \( \mathcal{M} \).

**Proof.** Denote by \( R \in \mathcal{R} \) the rigid motion for which the infimum in (2.1) is attained for \( \mathcal{C} \).

The first step in our proof is to derive a uniform bound on \( \| R(x) - C(x) \| \). We start by noting that the function \( q(x) = \| R(x) - C(x) \| \) is Lipschitz with a constant \( \lambda \) dependent only on \( \mathcal{M} \). Indeed, we have

\[
\| R(x) - C(x) \| - \| R(y) - C(y) \| \leq \| R(x) - R(y) \| + \| C(x) - C(y) \|
\]

\[
= \| x - y \| + \| C(x) - C(y) \|. \]

By assumption, \( d_{\mathcal{S}}(C(x), C(y)) \leq M d_{\mathcal{S}}(x, y) \). By Lemma 3.1, \( d_{\mathcal{S}}(x, y) \leq 3/2 \| x - y \| \) if \( d_{\mathcal{S}}(x, y) \) is sufficiently small. On the other hand, we have, for all \( x', y' \in \mathcal{S}' \), \( \| x' - y' \| \leq d_{\mathcal{S}}'(x', y') \), \( d_{\mathcal{S}}' \) is the metric
induced on $S'$ by the Euclidean metric in $\mathbb{R}^3$. Thus $\|C(x) - C(y)\| \leq 3M/2 \|x - y\|$ when $\|x - y\|$ is sufficiently small. Since on the other hand $S'$ is compact and thus bounded, $\|C(x) - C(y)\|$ is bounded uniformly in $x, y$ regardless of $\|x - y\|$. It follows that there exists a constant $\lambda$, depending only on the geometric properties of the surfaces $S$ and $S'$, and on $M$, such that

$$\left\| R(x) - C(x) \right\| - \left\| R(y) - C(y) \right\| \leq \lambda \|x - y\|.$$ 

Suppose $q$ attains its maximum $Q$ in $u \in S$. Set $\alpha = \min \left( \rho, \frac{Q}{2\lambda} \right)$, with $\rho > 0$ as in Lemma [3.4]. Then we must have

$$\int_{\{x \in S : \|u - x\| < \alpha\}} \max(0, Q - \lambda \|u - x\|)^2 \, d\text{vol}_S(x) \leq \int_{\{x \in S : \|u - x\| < \alpha\}} \|R(x) - C(x)\|^2 \leq d\rho(S, S'; C)^2 \leq \epsilon^2.$$ 

On the other hand, we also have, by Lemma [3.4] and using $Q - \lambda \|x - u\| \geq Q - \lambda \alpha$ on $\{x \in S : \|u - x\| < \alpha\}$,

$$\int_{\{x \in S : \|u - x\| < \alpha\}} \max(0, Q - \lambda \|u - x\|)^2 \, d\text{vol}_S(x) \geq \int_{\{x \in S : \|u - x\| < \alpha\}} (Q - \lambda \alpha)^2 \, d\text{vol}_S(x) = (Q - \lambda \alpha)^2 \int_{\{x \in S : \|u - x\| < \alpha\}} d\text{vol}_S(x) \geq \frac{Q^2}{4} \Gamma \alpha^2 = \frac{\Gamma}{4} Q^2 \min \left( \rho, \frac{Q}{2\lambda} \right)^2.$$ 

This implies, in particular, that

$$\frac{\Gamma}{4} Q^2 \min \left( \rho, \frac{Q}{2\lambda} \right)^2 \leq \epsilon^2.$$ 

If $Q/(2\lambda) > \rho$, then it follows that $\Gamma Q^2 \rho^2/4 < \epsilon^2$, hence (by using $Q/(2\lambda) > \rho$ once again) $\Gamma \lambda^2 \rho^4 < \epsilon^2$. Note that $\Gamma$, $\lambda$, and $\rho$ are constants that depend only on the geometrical bounds that we impose on $S$, $S'$ separately; a priori they bear no relationship to whether or not the continuous Procrustes distance between the surfaces is small. With a left hand side independent of $\epsilon$ and strictly positive, the inequality above can therefore not be satisfied if $\epsilon$ is sufficiently small; more precisely, if $\epsilon \leq \Gamma^{1/2} \lambda \rho^2$, then this case is excluded.

For sufficiently small $\epsilon$, we have thus $Q/(2\lambda) \leq \rho$, implying $\Gamma Q^4/(16\lambda^2) \leq \epsilon^2$, or $Q \leq 2 \lambda^{1/2} \Gamma^{-1/4} \epsilon^{1/2}$. In other words, there exists a constant $C_1 > 0$, dependent on only $\lambda$, $\rho$, $M$ and $\kappa$, such that, for sufficiently small $\epsilon$,

$$\max_{x \in S} \|R(x) - C(x)\| = Q \leq C_1 \epsilon^{1/2},$$

which is the desired uniform bound on $\|R(x) - C(x)\|$. Second, by Lemma [3.2] we can take $y \in \partial B_g(x, \epsilon^{1/4})$ such that

$$\frac{\|C(y) - C(x)\|}{\|x - y\|} = \|DC_x\|_{g,h} + O(\epsilon^{1/4}).$$

Using the triangle inequality as well as $\|R(x) - R(y)\| = \|x - y\|$, and applying Lemma [3.1] we obtain

$$\frac{\|C(y) - C(x)\|}{\|x - y\|} \leq \frac{\|C(y) - R(y)\| + \|x - y\| + \|R(x) - C(x)\|}{\|x - y\|} \leq 1 + O(\epsilon^{1/4}),$$

and thus

$$\|DC_x\|_{g,h} \leq 1 + O(\epsilon^{1/4}).$$

Lastly, since $\|DC_x\|_{g,h}$ equals the larger singular value of the matrix for $DC_x$ w.r.t. orthonormal bases of $T_xS$ and $T_{C(x)}S'$ (respectively), and since $C$ is area-preserving (implying that the determinant of this $2 \times 2$ matrix equals 1) the conformal distortion of $C$ at $x$ is $\|DC_x\|_{g,h}^2$, and thus

$$\text{dist}_C(x) \leq 1 + O(\epsilon^{1/4}).$$

□
Theorem 3.5 tells us that area-preserving diffeomorphisms associated to small surface Procrustes distances have small conformal distortion everywhere. We will next use the theory of quasi-conformal (QC) maps to see that, for disk-type surfaces, this implies that such maps then must be “close” to conformal maps.

For the sake of convenience, we restrict our discussion here to the case of disk-type surfaces here (similar results can be shown for sphere-type surfaces). More precisely, we start with two disk type surfaces $S, S' \subset \mathbb{R}^3$ with induced metric tensors $g, h$ (respectively), and we consider a global conformal parametrization (uniformization) of each onto their canonical domain, $\Psi : S \to D, \Psi' : S' \to D$. The surfaces are then intrinsically represented by their conformal factors $\mu$ and $\nu$. In other words, the push-forward metric tensors of $S, S'$ under the maps $\Psi, \Psi'$ are given by $(\Psi_* g)[z] = \mu(z) dzd\bar{z}$, and $(\Psi'_* h)[w] = \nu(w) dwd\bar{w}$, respectively. The conformal factors also act as “density functions” in the sense that the area in $S \subset \mathbb{R}^3$ of an arbitrary Borel set $\Omega \subset S$ can be written as $\text{vol}_S(\Omega) = \int_{\Psi(\Omega)} \mu(z) dzd\bar{z}$, where $z = x + iy$; similarly for the surface $S'$.

Now every conformal mapping from $S$ to $S'$ can be written as $\Psi^{-1} \circ m \circ \Psi$, where $m$ ranges over the Möbius transformations of the unit disk that preserve its boundary:

$$m(z) = e^{i\theta} \frac{z - a}{1 - z \bar{a}},$$

where $\theta \in [0, 2\pi)$, $a \in D$. This family of transformations has three degrees of freedom (one for the angle and two for the complex number $a$); we denote the family by $\text{Mob}(D)$.

Likewise an area preserving (and orientation preserving) map $\mathcal{C}$ from $S$ to $S'$ can be “transported” to $D$ by means of $\Psi$ and $\Psi'$, leading us to consider instead $\mathcal{C}_\alpha := \Psi' \circ \mathcal{C} \circ \Psi^{-1}$, mapping $D$ to itself. We will use QC theory to show that, if $d_P(S, S'; \mathcal{C})$ is small, then $\mathcal{C}_\alpha$ is close to an element of $\text{Mob}(D)$, with respect to the maximum norm over the unit disk $D = \{ z \in \mathbb{C} \mid |z| < 1 \}$, at least if $\mathcal{C}$ is orientation preserving. If it is orientation reversing, it is close to an anti-conformal map. We provide details below for the orientation preserving case; the reversing case is entirely similar.

By an appropriate Möbius change of coordinates $\tilde{m}$, replacing $\Psi$ by $\tilde{\Psi} = \tilde{m} \circ \Psi'$, we can even ensure that $\mathcal{C}_\alpha := \tilde{m} \circ \mathcal{C}_\alpha$ has 0 and 1 as fixed points. Abusing notation, and denoting $\mathcal{C}_\alpha$ by $\mathcal{C}$ again, we thus assume $\mathcal{C}(0) = 0$, and $\mathcal{C}(1) = 1$. We shall show that $\mathcal{C}$ is close to the identity, which means that $\mathcal{C}_\alpha$ is close to $\tilde{m}^{-1}$, and thus that the original area preserving map from $S$ to $S'$ is close to the conformal map from $S$ to $S'$ given by $(\Psi')^{-1} \circ \tilde{m}^{-1} \circ \Psi$.

We consider, as is very customary in complex analysis, derivatives with respect to $z$ and $\bar{z}$ of the differentiable map $\mathcal{C}$ from the subset $D$ of $\mathbb{C}$ to itself, i.e.

$$\frac{\partial \mathcal{C}}{\partial z} = \frac{\partial \mathcal{C}}{\partial x} - i \frac{\partial \mathcal{C}}{\partial y} \quad \text{and} \quad \frac{\partial \mathcal{C}}{\partial \bar{z}} = \frac{\partial \mathcal{C}}{\partial x} + i \frac{\partial \mathcal{C}}{\partial y}, \quad \text{where} \quad z = x + iy.$$

We define the complex dilation of $\mathcal{C}$ by

$$\varrho = \frac{\partial \mathcal{C}}{\partial \bar{z}} \Bigg/ \frac{\partial \mathcal{C}}{\partial z}.$$ 

For orientation preserving $\mathcal{C}$ we have (see for example, [1]):

$$\text{dis}_\mathcal{C} = \frac{1 + |\varrho|}{1 - |\varrho|}, \quad |\varrho| = \frac{\text{dis}_\mathcal{C} - 1}{\text{dis}_\mathcal{C} + 1}.$$

Theorem 3.5 therefore implies, uniformly on $D$,

$$\varrho = O(\varepsilon^{1/4}).$$

We will use the following existence and uniqueness theorem for the Beltrami equation (see [9], Theorem 4.30):

**Theorem 3.6.** For every $\varrho : \mathbb{C} \to \mathbb{C}$ measurable such that $\| \varrho \|_\infty < 1$, there exists a homeomorphism $f$ of $\mathbb{C}$ onto $\mathbb{C}$ which is a quasiconformal mapping of $\mathbb{C}$ with complex dilation $\varrho$. Moreover, $f$ is uniquely determined by the following normalization conditions: $f(0) = 0$, $f(1) = 1$, and $f(\infty) = \infty$. 
As is customary, we will call normalized solution any solution of a Beltrami equation that satisfies the normalization conditions.

Theorem 3.6 requires the complex dilation \( \rho \) to be defined on all of \( \mathbb{C} \). Before applying it, we thus need to first obtain \( \rho \) on all of \( \mathbb{C} \), which we do by extending \( \mathbb{C} \) from \( \mathcal{D} \) to the entire complex plane \( \mathbb{C} \) by reflection:

\[
\hat{\mathcal{C}}(z) = \begin{cases} 
\mathcal{C}(z) & |z| \leq 1 \\
1/\mathcal{C}(1/\bar{z}) & |z| > 1
\end{cases}
\]

Note that the extension \( \hat{\mathbb{C}} \) is normalized, that is, it satisfies \( \hat{\mathbb{C}}(0) = 0, \hat{\mathbb{C}}(1) = 1, \hat{\mathbb{C}}(\infty) = \infty \). Moreover, this extension preserves the conformal distortion, that is, for \( |z| > 1 \):

\[
dis_{\hat{\mathcal{C}}}(z) = dis_{\mathcal{C}}(1/\bar{z}).
\]

It follows that this extension of \( dis_{\mathcal{C}} \) to all of \( \mathbb{C} \) still satisfies (3.3). We now have

\[
\text{Lemma 3.7. The extension } \hat{\mathcal{C}} : \mathbb{C} \to \mathbb{C} \text{ is the unique normalized solution to the following Beltrami equation:}
\]

\[
\hat{\mathcal{C}}z(\hat{\mathcal{C}}z) = \hat{\varrho}(z) \hat{\mathcal{C}}z(\hat{\mathcal{C}}z),
\]

where \( \hat{\varrho} \) is a complex dilation (a.k.a. Beltrami coefficient) defined by

\[
\hat{\varrho}(z) = \begin{cases} 
\varrho(z) & |z| < 1 \\
0 & |z| = 1 \\
\varrho(1/\bar{z}) (z^2/\bar{z}^2) & z \in |z| > 1
\end{cases}
\]

\[
\text{Proof. A straightforward calculation shows that } \hat{\mathcal{C}} \text{ has the Beltrami coefficient } \hat{\varrho} \text{ almost everywhere. As mentioned above, } \hat{\mathcal{C}} \text{ satisfies the normalization conditions of Theorem 3.6 and therefore the uniqueness follows from Theorem 3.6.} \]

We will next use Proposition 4.36 from [9], the statement of which is:

\[
\text{Theorem 3.8. If } \|\varrho\|_\infty \to 0, \text{ then the normalized solution of the Beltrami equation } f^\varrho \text{ converges to the identity in the maximum norm on } \mathcal{D}, \|f^\varrho - Id\|_\infty \to 0, \text{ where } Id(z) = z.
\]

The proof of Proposition 4.36 in [9] actually demonstrates a slightly stronger claim:

\[
\text{Theorem 3.9. If } \|\varrho\|_\infty \to 0, \text{ then the normalized solution of the Beltrami equation } f^\varrho \text{ satisfies}
\]

\[
\|f^\varrho - Id\|_\infty \leq M \|\varrho\|_\infty,
\]

on \( \mathcal{D} \), for some constant \( M > 0 \) independent of sufficiently small \( \varrho \).

Combining Theorems 3.6 and 3.9 finally yields

\[
\text{Theorem 3.10. Let } S, S' \subset \mathbb{R}^3 \text{ be 2-manifolds with induced Riemannian metrics } g, h \text{ (respectively), with curvatures bounded above by } \kappa, \text{ and satisfying the } (\sigma, \theta)-\text{cone condition. We consider area-preserving and orientation-preserving diffeomorphisms } \mathcal{C} : S \to S' \text{ with first and second order differentials bounded by } M.
\]

Let \( \Psi : S \to \mathcal{D}, \Psi' : S' \to \mathcal{D} \) be uniformizing maps of \( S, S' \) onto the disk. Let \( m \) be a disk-preserving Möbius transformation such that \( f = m \circ \Psi' \circ \mathcal{C} \circ \Psi^{-1} : \mathcal{D} \to \mathcal{D} \) satisfies \( f(0) = 0, f(1) = 1 \). Then the bound \( d_P(S, S', \mathcal{C}) \leq \epsilon \) implies the following bound:

\[
\|f - Id\|_\infty = O(1/\epsilon),
\]

where \( Id(z) = z \) is the identity map, and where the constant in the \( O \)-notation depends on only \( \kappa, \sigma, \theta \) and \( S \).
Figure 2. A surface (left) and its density function over the uniformization disk. The local extremas of the conformal density function are shown as black dots.

The orientation reversing \( C : S \to S' \) are close to the anti-Möbius transformations that can be calculated from the Möbius transformations by setting

\[
m(z) = m(\bar{z}),
\]

where \( m \) is any Möbius transformation.

As described earlier, we use this theorem as a guide to build an efficient search algorithm to compute (an approximation to) \( d_P(S, S') \) for surfaces \( S, S' \) that are not hugely dissimilar. Since area-preserving maps \( C \) from \( S \) to \( S' \) that are close to minimizing \( d_P(S, S'; C) \) must be close to conformal, we start by searching \( \text{Mob}(S, S') \) to find the conformal or anti-conformal map \( m \) that minimizes \( d_P(S, S'; m) \). We then transform this \( m \) into a nearby area-preserving diffeomorphism by means of a nonlinear transform \( \text{Pr} \), still to be defined below. We expect (but do no prove) that \( \text{Pr}(m) \) is then a good approximation to (nearly) minimizing \( C \).

Note that there are no guarantees that this approximation process, in which we replace \( A(S, S') \) by the proxy \( \text{Pr}(\text{Mob}(S, S')) \), preserves the triangle inequality property of \( D_{cP}(S, S') \); the approximations we compute therefore result in a measure of dissimilarity rather then a distance.

4. Searching appropriate Möbius candidates and massaging them into area-preservation

In the previous section we showed that it is useful to first find a Möbius transformation \( m \) for which \( d_P(S, S'; m) \) is small; we show in subsection 4.1 below a practical strategy for obtaining such candidate Möbius transformations that is fast and efficient for our applications. To obtain a better approximation of the optimal element of \( A(S, S') \) from these candidate \( m \in \text{Mob}(S, S') \), we will, in subsections 4.2 and 4.3, deform each of them into a nearby area-preserving map. That is, for every \( m \in \text{Mob}(S, S') \), we will construct a map \( f_m : S \to S' \) such that \( f_m \circ m \in A(S, S') \).

4.1. Searching the Möbius group. By Theorem 3.10 we know that an area-preserving diffeomorphism \( C : S \to S' \) that produces a small continuous Procrustes distance \( d_P(S, S'; C) \), is close to a Möbius transformation, when written in uniformizing coordinates. Hence, we first describe how we search for candidate Möbius transformations \( m \in \text{Mob}(S, S') \) that (we hope) are already close to area-preserving for our applications. As mentioned above, the Möbius group between two disk-type surfaces has three real degrees of freedom: prescribing the image \( w_0 \in D \) of one point \( z_0 \in D \), as well as one angle \( \theta \in [0, 2\pi) \), uniquely defines a disk-preserving Möbius transformation \( m : D \to D \). To speed up the search, we start by determining a mapping for which the density peaks, i.e. the local extrema of the density \( \mu(m(z)) \) (more or less) correspond to those of \( \mu(z) \). To that end we first extract, for each surface, a set of extremal points \( I_S, I_{S'} \) (local maxima and minima) defined by local extrema of the corresponding density functions \( \mu, \nu \), respectively. See Figure 2 where the black points show these extremal sets. In practice, we find that, in the application (to
bone surfaces) that first motivated us; these points (intimately related to extrema of Gauss curvature) were likely to contain at least one pair of corresponding points, across a wide range of examples; this feature has persisted for other families of examples we examined. Note that this definition of $I_S, I_{S'}$ is not invariant to Möbius transformations in the sense that for any Möbius transformation the extrema of the pulled-back density $\nu(m(z)) |m'(z)|^2$ are not, in general, the same as the $m^{-1}(w_t)$, where the $w_t$ are the extrema of $\nu(w)$. To make the computation invariant it is sufficient to search for the extrema of the hyperbolic normalized densities $(1 - |z|^2)^2 \mu(z)$ and $(1 - |w|^2)^2 \nu(w)$ (which are invariant to Möbius change of coordinates).

In our algorithm we consider the collection of Möbius transformations $m = m(z; \theta, p, q)$ defined by $m(p) = q$ for every pair $(p, q) \in I_S \times I_{S'}$, and every angle $\theta \in [0, 2\pi)$. In order to compute the Möbius transformations in practice between two surfaces, we use the algorithm described in [11, 12]. Furthermore, we discretize distances in a mass-transportation approach, but this is a much more challenging project, which we intend to tackle in future work.

Other researchers have used Moser’s technique to construct an initial guess in the further elaboration of an area-preserving map that would be optimal in the sense of mass-transportation cost [5]. Although Monge’s mass-transportation provides a elegant way to construct correspondence maps, we believe that, because Euclidean (or hyperbolic) distances in the uniformization plane have no intrinsic meaning for the geometry of the problem, using them in the present context will not give a more meaningful answer than the straightforward result of Moser’s procedure. More meaningful would be to use the surfaces’ induced geodesic distances in a mass-transportation approach, but this is a much more challenging project, which we intend to tackle in future work.

Since our measures are absolutely continuous w.r.t to the Lebesgue measures $dz, dw$ respectively, we write $d\mu = \mu(z) dz, d\nu = \nu(w) dw$, using the conformal factors $\mu(z), \nu(w)$ as densities. Using the standard change of variables formula we see that (4.1) can be rewritten, in terms of the densities, as

\[
(\phi_m)_* d\mu = d\nu.
\]

We will be interested in a solution to (4.2) that is a diffeomorphism $\phi_m$ of $D$ onto itself; in particular points on the boundary of the unit disk should be mapped to the boundary again. For the remainder of this subsection we will drop the subscript on $\phi_m$, writing it as $\phi$ for brevity.
Adapting Dacorogna and Moser’s procedure \cite{2} we define the diffeomorphism $\phi$ by integrating, for $t \in [0, 1]$, a special time dependent vector field $v_t(z)$ (to be defined below):

$$
\frac{d}{dt} \Phi_t(z) = v_t(\Phi_t(z)), \quad \text{for all } t \geq 0, \ z \in \mathcal{D} \tag{4.3}
$$

$$
\Phi_0(z) = z, \quad \text{for all } z \in \mathcal{D}. \tag{4.4}
$$

The desired map $\phi$ is then the end result of the integration, $\phi(z) = \Phi_1(z)$. The vector field $v_t$ is defined in three steps, as follows. We start by solving a Poisson equation with Neumann boundary conditions,

$$
\Delta a = \mu - \nu, \quad \text{in } \mathcal{D} \tag{4.5}
$$

$$
\frac{\partial a}{\partial n} = 0, \quad \text{on } \partial \mathcal{D}. \tag{4.6}
$$

[Note that, unlike Dacorogna and Moser we do not require $\phi(z) = z$ for $z \in \partial \mathcal{D}$; we impose only that the boundary of $\mathcal{D}$ be mapped to the boundary – hence the use of Neumann instead of Dirichlet boundary conditions.] Next, a time-independent vector field $v$ is defined by setting $v(z) = \nabla a(z)$. In the third step, we define the time-dependent vector field $v_t$ as

$$
v_t(z) = \frac{v(z)}{t \cdot \nu(z) + (1-t) \cdot \mu(z)}. \tag{4.7}
$$

Establishing that $\phi(z) = \Phi_1(z)$ provides a solution to (4.2) can be done by adapting Dacorogna and Moser’s original proof. For completeness let us briefly describe the argument. First, we define an auxiliary function:

$$
\lambda(t, z) = \left( \text{det } \nabla \Phi_t(z) \right) \left( t \cdot \nu(\Phi_t(z)) + (1-t) \cdot \mu(\Phi_t(z)) \right); \tag{4.8}
$$

as we shall see below, this function satisfies

$$
\frac{\partial}{\partial t} \lambda(t, z) = 0. \tag{4.9}
$$

For the time derivative of the first factor we refer to \cite{2}:

$$
\frac{\partial}{\partial t} (\text{det } \nabla \Phi_t(z)) = \text{det } \nabla \Phi_t(z) \cdot \text{div } v_t(\Phi_t(z)). \tag{4.10}
$$

Differentiating (4.7) w.r.t. time gives thus

$$
\frac{\partial}{\partial t} \lambda(t, x) = \text{det } \nabla \Phi_t \cdot \text{div } v_t(\Phi_t) \cdot \left( t \cdot \nu(\Phi_t) + (1-t) \cdot \mu(\Phi_t) \right)
$$

$$
+ \text{det } \nabla \Phi_t \left( \nu(\Phi_t) - \mu(\Phi_t) + (t \nabla \nu(\Phi_t) + (1-t) \nabla \mu(\Phi_t), \frac{d}{dt} \Phi_t) \right). \tag{4.11}
$$

By the definition of $v_t$ we obtain

$$
\text{div } v = (\text{div } v_t) (t \cdot \nu + (1-t) \cdot \mu) + (t \nabla \nu + (1-t) \nabla \mu, v_t). \tag{4.12}
$$

Together with (4.3) this leads to several cancellations in (4.10), resulting in

$$
\frac{\partial}{\partial t} \lambda(t, z) = \text{det } \nabla \Phi_t \left( \text{div } v(\Phi_t) + (\nu(\Phi_t) - \mu(\Phi_t)) \right). \tag{4.13}
$$

Since $\nu$ is defined as $\nabla a$, and $a$ satisfies (4.5), this implies (4.8). Therefore,

$$
\lambda(0, z) = \lambda(1, z). \tag{4.14}
$$

Because $\Phi_0(z) = z$, we have $\lambda(0, z) = \mu(z)$, so that we have shown that

$$
\mu(z) = \text{det } \nabla \Phi_1(z) \nu(\Phi_1(z)). \tag{4.15}
$$

Finally, it is clear from the Neumann boundary conditions (4.6) that the vector field $v(z)$ and therefore $v_t(z)$ is tangent to the unit circle at the boundary of the unit disk, that is $\langle v_t(z), z \rangle = 0$ for all $z \in \partial \mathcal{D}$ and $t \geq 0$. This property ensures that integral curves $\Phi_t(z)$ for $z \in \partial \mathcal{D}$ will stay on the boundary of the disk for all times $t \geq 0$. 

Implementation details: We used the MATLAB\textsuperscript{TM} PDE TOOLBOX for all steps. For the first step (solving the Poisson equation) we used a triangular mesh with regular mesh size. The two densities are taken to be piecewise constant on the elements, with constants given by evaluating \( \mu \) and \( \nu \) at the midpoints of the triangles, providing the right-hand side of the PDE. Since the solution \( a \) of the PDE is also piecewise constant on the mesh elements, its gradient field \( \nabla a \) can be determined on each node of the mesh. By a nearest neighbor interpolation we approximate \( \nu \) as piecewise constant on the elements and use this to solve the ODE in the second step. This is done with a 4-stage Runge-Kutta method. Another implementation detail is that we add a small constant to the densities to avoid numerical inabilities for densities that have a minimal value close to zero.

4.3. Thin-Plate Splines deformation. From a practical point of view we found it desirable to define our projection map as a composition of two maps: \( I_m = \phi_m \circ \zeta_m \), combining the Moser map \( \phi_m \) defined above with a preliminary smooth planar deformation \( \zeta_m \). The map \( \zeta_m \) is used to locally align the peaks and valleys, already brought close together by the Möbius transformation \( m \). Since we assume the two surfaces have equal (unit) area, i.e., \( \int_S d\text{vol}_S(x) = 1 = \int_S d\text{vol}_S(y) \), improving the alignment of peaks and valleys of the densities leads to less area distortion. This quick-and-dirty approximation jumpstarts the transition towards an exact area-preservation; although true area-preservation is achieved only after the second step of the deformation, an initial alignment by means of \( \zeta_m \) removes some of the “workload” on \( \phi_m \).

For the smooth deformation \( \zeta_m \), we use Thin-Plate Splines (TPS). In a first step, we label the points in \( I_S \) and \( I_{S'} \) as follows. We first apply \( m \) to the set \( I_S \), determine mutually closest points (with respect to the hyperbolic distance function) for the two sets \( m(I_S) \) and \( I_{S'} \), and label them correspondingly, so that \( (p_j, q_j) \in m(I_S) \times I_{S'}, \ j = 1, \ldots, n \), denote the mutually closest pairs. In other words, we have

\[
d_H(p_j, q_j) < \min \left\{ \min_{q_j \neq q \in I_{S'}} d_H(p_j, q), \min_{p_j \neq p \in I_S} d_H(p, q_j) \right\},
\]

where the hyperbolic distance is \( d_H(p, q) = \tanh^{-1} \left| \frac{p-q}{1-p \cdot q} \right|, \ p, q \in D \).

Next, we carry out a change of coordinates that maps the unit disk to the whole plane, by setting \( \chi(z) = \text{atan}(|z|) z / |z| \) with the inverse \( \chi^{-1}(z) = \tan(|z|) z / |z| \). Set \( P_j = \chi(p_j), Q_j = \chi(q_j), \ j = 1, \ldots, n \). We construct a thin-plate spline function \( \zeta_m \) interpolating the \( P_j \) and \( Q_j \) in the complex plane, i.e., \( \zeta_m(P_j) = Q_j \).

More explicitly,

\[
\zeta_m(z) = \chi^{-1} \circ TPS_m \circ \chi,
\]

where

\[
TPS_m(z) = a_0 + a_1 z + a_2 \bar{z} + \sum_{i=1}^n b_i \Upsilon(|z - P_j|),
\]

and \( \Upsilon(r) = r^2 \log(r) \). The coefficients \( a_j, b_i, j = 0, 1, 2, i = 1, \ldots, n \) are computed in the standard way by solving an \((n+3) \times (n+3)\) linear system [15] that imposes \( TPS_m(P_j) = Q_j, \ j = 1, \ldots, n \). “Sandwiching” \( TPS_m \) by the coordinate transformation \( \chi \) guarantees that \( \zeta_m \) takes the disk \( D \) onto itself.

4.4. Numerical experiments. Figures 3 and 4 demonstrate different aspects of the behavior of the algorithm described in the earlier sections.

In the companion paper [4] an extensive analysis is performed for three biological data-sets, comparing the results of several algorithms to define the (dis)similarity between surfaces with those obtained by human experts. One of the methods illustrated in [4] uses the algorithm described here, and we refer the interested reader to that paper for many more figures and results. (In the interest of full disclosure, we confess that in many of the examples in [4] that used continuous Procrustes distances, we skipped the last step in \( Pr \): the combination of an optimal Möbius transformation and TPS already gave results that were very close to area-preserving, and sufficed for the application at hand, so that we could skip the more time-consuming Moser transformation.)
Figure 3. **Mesh deformation under Moser’s procedure.** Left: a “jiggled” initial mesh; Right: its deformation after solving the PDE on this mesh.

Figure 4. **The different components of the map.** The left column shows the surface $S'$ (top, with colored squares enabling the viewer to track where different portions of the surface $S$ are mapped), and the corresponding conformal factor $\nu$ on the disk $D$. The different steps of the algorithm “at work” in constructing the map $C$ from $S$ to $S'$ are shown to the right of the vertical black line. From left to right: the optimal Möbius transformation $m$, which gives a uniformization of $S$, with conformal factor $\mu$; the optimal alignment of the peaks in $\mu$, via TPS, with those of $\nu$; the transformation into a truly area-preserving map via Moser’s technique.

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