On the Meaning of Mean Shape

Stephan F. Huckemann

Abstract
Various concepts of mean shape previously unrelated in the literature are brought into relation. In particular for non-manifolds such as Kendall’s 3D shape space, this paper answers the question, for which means one may apply a two-sample test. The answer is positive if intrinsic or Ziezold means are used. The underlying general result of manifold stability of a mean on a shape space, the quotient due to an isometric action of a compact Lie group on a Riemannian manifold, blends the Slice Theorem from differential geometry with the statistics of shape. For 3D Procrustes means, however, a counterexample is given. To further elucidate on subtleties of means, for spheres and Kendall’s shape spaces, a first order relationship between intrinsic, residual/Procrustean and extrinsic/Ziezold means is derived stating that for high concentration the latter approximately divides the (generalized) geodesic segment between the former two by the ratio 1 : 3. This fact, consequences of coordinate choices for the power of tests and other details, e.g. that extrinsic Schoenberg means may increase dimension are discussed and illustrated by simulations and exemplary datasets.

Key words and phrases: intrinsic mean, extrinsic mean, Procrustes mean, Schoenberg mean, Ziezold mean, shape spaces, compact Lie group action, slice theorem, horizontal lift, manifold stability

Figure AMS 2000 Subject Classification: Primary 60D05
Secondary 62H11

1 Introduction

The analysis of shape may be counted among the very early activities of mankind; be it for representation on cultural artefacts, or for morphological, biological and medical applications. In modern days shape analysis is gaining increased momentum in computer vision, image analysis, biomedicine and many other fields. For a recent overview cf. [Krim and Yezzi (2006)].

A shape space can be viewed as the quotient of a Riemannian manifold – e.g. the pre-shape sphere of centered unit size landmark configurations – modulo the isometric and proper action of a Lie group (cf. Bredon (1972)), conveying shape equivalence – e.g. the group of rotations, cf. (Kendall et al. 1999, Chapter 11). Thus, it carries the canonical quotient structure of a union
of manifold strata of different dimensions, which give in general a Riemannian manifold part – possibly with singularities comprising the non-manifold part of non-regular shapes at some of which sectional curvatures may tend to infinity, cf. (Kendall et al. 1999, Chapter 7.3) as well as [Huckemann et al. 2010b].

In a Euclidean space, there is a clear and unique concept of a mean in terms of least squares minimization: the arithmetic average. Generalizing to manifolds, however, the concept of expectation, average or mean is surprisingly non trivial and not at all canonical. In fact, it resulted in an overwhelming number of different concepts of means, each defined by a specific concept of a distance, all of which are identical for the Euclidean distance in a Euclidean space. More precisely, with every embedding in a Euclidean space come specific extrinsic and residual means and with every Riemannian structure comes a specific intrinsic mean. Furthermore, due to the non-Euclidean geometry, local minimizers introduced as Karcher means by Kendall (1990) may be different from global minimizers called Fréchet means by Ziezold (1977), and, neither ones are necessarily unique. Nonetheless, carrying statistics over to manifolds, strong consistency (by Ziezold (1977), Bhattacharya and Patrangenaru (2003)) and under suitable conditions, central limit theorems (CLTs) for such means have been derived (by Jupp (1988), Hendriks and Landsman (1996, 1998), Bhattacharya and Patrangenaru (2003) as well as Huckemann (2010a)). On shape spaces, various other concepts of means have been introduced, e.g. the famous Procrustes means (cf. Ziezold (1977), Dryden and Mardia (1998)). As we show here, these means are related to the above ones via a horizontal lifting from the bottom quotient to the top manifold, cf. Table 1. In particular, since there are many – and often confusing – variants of Procrustes means in the literature this paper introduces the terminology of Procrustean means standing for inheritance from residual means.

| manifold means | shape means |
|----------------|-------------|
| intrinsic      | intrinsic   |
| extrinsic      | Ziezold     |
| residual       | Procrustean |

Table 1: Three fundamental types of means on a shape space (right column) and their horizontal lifts to the respective manifold (left column).

For a CLT to hold, a manifold structure locally relating to a Euclidean space is sufficient. This leads to the question under which conditions it can be guaranteed that a mean shape lies on the manifold part.

Due to strong consistency, for a one-sample test for a specific mean shape on the manifold part, it may be assumed that sample means eventually lie on the manifold part as well, thus making the above cited CLTs available. To date however, a two- and a multi-sample test could not be justified because of a lacking result on the following manifold stability.

Definition 1.1. A mean shape enjoys manifold stability if it is assumed on the
manifold part for any random shape assuming the manifold part with non-zero probability.

A key result of this paper establishes manifold stability for intrinsic and Ziezold means under the following condition.

**Condition 1.2.** On the non-manifold part the distribution of the random shape contains at most countably many point masses.

Since the non-manifold part is a null-set (e.g. Bredon (1972)) under the projection of the Riemannian volume, this condition covers most realistic cases.

We develop the corresponding theory for a general shape space quotient based on lifting a distribution on the shape space to the pre-shape space and subsequently exploiting the fact that intrinsic means are zeroes of an integral involving the Riemann exponential. The similar argument can be applied to Ziezold means but not to Procrustean means. More specifically, we develop the notion of a *measurable horizontal lift* of the shape space except for its *quotient cut locus* (introduced as well) to the pre-shape space. This requires the geometric concept of *tubular neighborhoods admitting slices*.

Curiously, the result applied to the finite dimensional subspaces exhausting the quotient shape space of closed planar curves with arbitrary initial point introduced by Zahn and Roskies (1972) and further studied by Klassen et al. (2004), gives that the shape of the circle, since it is a singularity, can never be an intrinsic shape mean of non-circular curves.

As a second curiosity, 3D full Procrustes means do not enjoy manifold stability in general, a counterexample involving low concentration is given. This is due to the fact that for low concentration, full Procrustes means may be ‘blinder’ in comparison to intrinsic and Ziezold means to distributional changes far away from a mode. Included in this context is also a discussion of the Schoenberg means, recently introduced by Bandulasiri and Patrangenaru (2005) as well as by Dryden et al. (2008) for the non-manifold Kendall reflection shape spaces, which in the ambient space, also allow for a CLT. Schoenberg means, as demonstrated, however, may feature ‘blindness’ in comparison to intrinsic and Ziezold means, with respect to changes in the distribution of nearly degenerate shapes. In a simulation we show that these features render Schoenberg means less effective for a discrimination involving degenerate or nearly degenerate shapes.

As a third curiosity, for spheres and Kendall’s shape spaces, it is shown that, given uniqueness, with order of concentration, the (generalized) geodesic segment between the intrinsic mean and the residual/Procrustean mean is in approximation divided by the extrinsic/Ziezold mean by the ratio $1:3$. This first order relationship can be readily observed in existing data sets. In particular, this result supports the conjecture that Procrustean means of sufficiently concentrated distributions enjoy stability as well.

This paper is structured as follows. For convenience of the reader, first in Section 2 Kendall’s shape spaces are introduced along with the specific result on manifold stability, followed by a classification of concepts of means on general shape spaces in Section 3. The rather technical Section 4 develops horizontal
lifting and establishes manifold stability, technical proofs are deferred to the appendix. In Section 5 extrinsic Schoenberg means are discussed and Section 6 tackles local effects of curvature on spheres and Kendall’s shape spaces. Section 7 illustrates practical consequences using classical data-sets as well as simulations. Note that lacking stability does not affect the validity of the Strong Law, on which the considerations on asymptotic distance in Sections 6 and 7 are based.

An R-package for all of the computations performed is provided online: [Huckemann (2010b)](https://example.com).

## 2 Stability of Means on Kendall’s Shape Spaces

In the statistical analysis of similarity shapes based on landmark configurations, geometrical $m$-dimensional objects (usually $m = 2, 3$) are studied by placing $k > m$ landmarks at specific locations of each object. Each object is then described by a matrix in the space $M(m,k)$ of $m \times k$ matrices, each of the $k$ columns denoting an $m$-dimensional landmark vector. $\langle x, y \rangle := \text{tr}(xy^T)$ denotes the usual inner product with norm $\|x\| = \sqrt{\langle x, x \rangle}$. For convenience and without loss of generality for the considerations below, only centered configurations are considered. Centering can be achieved by multiplying with a sub-Helmer matrix $H \in M(k,k-1)$ from the right, yielding a configuration $xH$ in $M(m,k-1)$. For this and other centering methods cf. [Dryden and Mardia, 1998, Chapter 2]. Excluding also all configurations with all landmarks coinciding gives the space of configurations

$$F^k_m := M(m,k-1) \setminus \{0\}.$$ 

Since only the similarity shape is of concern, we may assume that all configurations are contained in the unit sphere $S^k_m := \{x \in F^k_m : \|x\| = 1\}$ called the pre-shape sphere. Then, Kendall’s shape space is the canonical quotient

$$\Sigma^k_m := S^k_m / SO(m) = \{[x] : x \in S^k_m\}$$ with the orbit $[x] = \{gx : g \in SO(m)\}$.

In some applications reflections are also filtered out giving Kendall’s reflection shape space

$$R\Sigma^k_m := \Sigma^k_m / \{e, \tilde{e}\} = S^k_m / O(m).$$

Here, $O(m) = \{g \in M(m,m) : g^T g = e\}$ denotes the orthogonal group with the unit matrix $e = \text{diag}(1, \ldots, 1)$, $\tilde{e} = \text{diag}(-1, 1, \ldots, 1)$ and $SO(m) = \{g \in O(m) : \det(g) = 1\}$ is the special orthogonal group.

For $1 \leq j < m < k$ consider the isometric embedding

$$S^k_j \hookrightarrow S^k_m : x \mapsto \left(\begin{array}{c} x \\ 0 \end{array}\right)$$  \hspace{1cm} (1)

giving rise to a canonical embedding $R\Sigma^k_j \hookrightarrow \Sigma^k_m$ which is isometric w.r.t. the canonical intrinsic distance, the Procrustean distance and the Ziezold distance,
respectively, defined in Section 3, cf. (Kendall et al., 1999, p. 29), cf. also Remark 2.3 below.

We say that a configuration in $\mathbb{R}^m$ is $j$-dimensional, or more precisely non-degenerate $j$-dimensional if its preshape $x \in S^k_m$ is of rank $j$. Moreover, for $j \geq 3$ the shape spaces $\Sigma_j^k$ and $R\Sigma_j^k$ decompose into a manifold part (defined in Section 3, cf. also Section 5) of regular shapes $(\Sigma_j^k)^* = \{ [x] \in \Sigma_j^k : \text{rank}(x) \geq j-1 \}$ and $(R\Sigma_j^k)^* = \{ [x] \in R\Sigma_j^k : \text{rank}(x) = j \}$, respectively, given by the shapes corresponding to configurations of at least dimension $j-1$ and $j$, respectively and a non void part of singular shapes corresponding to lower dimensional configurations, respectively.

The following Theorem for intrinsic means, full Procrustes means and Ziezold means (also defined in Section 3) of random elements taking values in $R\Sigma_j^k$ follows from Proposition 3.3, Remark 6.8 and the fact that $R\Sigma_j^k \subset \Sigma_j^k$ contains all shapes in $\Sigma_j^k$ of configurations of dimension up to $j$, $1 \leq j < m < k$.

**Theorem 2.1.** Suppose that $X$ is a random shape on $\Sigma_j^k$ assumes shapes in $R\Sigma_j^k$ ($1 \leq j < m < k$) with probability one. Then every full Procrustes mean shape of $X$ and every unique intrinsic or Ziezold mean shape under Condition 1.2 w.r.t. $(R\Sigma_j^k)^*$ corresponds to a configuration of dimension less than or equal to $j$.

The following theorem is the application of the key result applied to Kendall’s shape spaces.

**Theorem 2.2** (Stability Theorem for Intrinsic and Ziezold means). Let $X$ be a random shape on $\Sigma_j^k$, $0 < m < k$, with unique intrinsic or Ziezold mean shape $[\mu] \in \Sigma_j^k$, $\mu \in S^k_m$ and let $1 \leq j \leq m$ be the maximal dimension of configurations of shapes assumed by $X$ with non-zero probability. Suppose moreover that shapes of configurations of strictly lower dimensions are assumed with at most countably many point masses.

(i) If $j < m$ then $\mu$ corresponds to a non-degenerate $j$-dimensional configuration.

(ii) If $j = m$ then $\mu$ corresponds to a non-degenerate configuration of dimension $m-1$ or $m$.

**Proof.** Lemma 4.1 teaches that for Kendall’s shape spaces, all quotient cut loci are void. Since for Ziezold means, Remark 3.5 provides invariant optimal positioning and Remark 4.2 provides the validity of (5), Corollary 4.8 applied to $R\Sigma_j^k$ as well as to $\Sigma_j^k$ states that intrinsic and Ziezold means are also assumed on the manifold parts of $R\Sigma_j^k$ and $\Sigma_j^k$, respectively. In conjunction with Theorem 2.1 this gives the assertion.  

**Remark 2.3.** The result of Theorem 2.2 is sharp. To see this, consider for $\alpha > \beta > 0$, $\alpha^2 + \beta^2 = 1$ the pre-shapes

$$x = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \end{pmatrix}, \quad y = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & 0 & -\beta \end{pmatrix} \quad \text{and} \quad z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \in S^2_2.$$
Then \(x\) and \(y\) correspond to non-degenerate two-dimensional quadrilateral configurations while \(z\) corresponds to a one-dimensional (collinear) quadrilateral. Still, \([z]\) is regular in \(\Sigma^2_2\) and it is the intrinsic and Ziezold mean of \([x]\) and \([y]\) in \(\Sigma^4_2\). Under the embedding \(R\Sigma^4_2 \rightarrow \Sigma^4_3\) we have the pre-shapes

\[
x' = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad y' = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & -\beta & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad z' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \in S^4_3.
\]

Just as \([x]\) = \([y]\) in \(R\Sigma^4_2\) so do \(x'\) and \(y'\) have regular and identical shape in \(\Sigma^4_3\). However, \([z']\) is not regular and it is not the intrinsic or Ziezold mean in \(\Sigma^4_3\).

3 Fundamental Types of Means

In the previous section we introduced Kendall’s shape and reflection shape space based on invariance under similarity transformations and, including reflections, respectively. Invariance under congruence transformations only leads to Kendall’s size-and-shape space. More generally in image analysis, invariance may also be considered under the affine or projective group, cf. Mardia and Patrangenaru (2001, 2005). A different yet also very popular popular set of shape spaces for two-dimensional configurations modulo the group of similarities has been introduced by Zahn and Roskies (1972). Instead of building on a finite dimensional Euclidean matrix space modeling landmarks, the basic ingredient of these spaces modeling closed planar unit speed curves is the infinite dimensional Hilbert space of Fourier series, cf. Klassen et al. (2004). In practice for numerical computations, only finitely many Fourier coefficients are considered.

To start with, a shape space is a metric space \((Q, d)\). For this entire paper suppose that \(X, X_1, X_2, \ldots\) are i.i.d. random elements mapping from an abstract probability space \((\Omega, \mathcal{A}, P)\) to \((Q, d)\) equipped with its self understood Borel \(\sigma\)-field. Here and in the following, measurable will refer to the corresponding Borel \(\sigma\)-algebras, respectively. Moreover, denote by \(\mathbb{E}(Y)\) the classical expected value of a random vector \(Y\) on a \(D\)-dimensional Euclidean space \(\mathbb{R}^D\), if existent.

Definition 3.1. For a continuous function \(\rho : Q \times Q \rightarrow [0, \infty)\) define the set of population Fréchet \(\rho\)-means by

\[
E^{(\rho)}(X) = \arg\min_{\mu \in Q} \mathbb{E}(\rho(X, \mu)^2).
\]

For \(\omega \in \Omega\) denote the set of sample Fréchet \(\rho\)-means by

\[
E_n^{(\rho)}(\omega) = \arg\min_{\mu \in Q} \sum_{j=1}^n \rho(X_j(\omega), \mu)^2.
\]

By continuity of \(\rho\), the \(\rho\)-means are closed sets, additionally, sample \(\rho\)-means are random sets, all of which may be empty. For our purpose here, we rely on the definition of random closed sets as introduced and studied by Choquet (1954), Kendall (1974) and Matheron (1975). Since their original definition for \(\rho = d\) by Fréchet (1948) such means have found much interest.
Intrinsic means. Independently, for a connected Riemannian manifold with geodesic distance \( \rho^{(i)} \), Kobayashi and Nomizu (1969) defined the corresponding means as centers of gravity. They are nowadays also well known as intrinsic means by Bhattacharya and Patrangenaru (2003, 2005).

Extrinsic means. W.r.t. the chordal or extrinsic metric \( \rho^{(e)} \) due to an embedding of a Riemannian manifold in an ambient Euclidean space, Fréchet \( \rho \)-means have been called mean locations by Hendriks and Landsman (1996) or extrinsic means by Bhattacharya and Patrangenaru (2003).

More precisely, let \( Q = M \subset \mathbb{R}^D \) be a complete Riemannian manifold embedded in a Euclidean space \( \mathbb{R}^D \) with standard inner product \( \langle x, y \rangle \), \( \|x\| = \sqrt{\langle x, x \rangle} \), \( \rho^{(e)}(x, y) = \|x - y\| \) and let \( \Phi : \mathbb{R}^D \to M \) denote the orthogonal projection, \( \Phi(x) = \arg\min_{p \in M} \|x - p\| \). For any Riemannian manifold an embedding that is even isometric can be found for \( D \) sufficiently large, see Nash (1956). Due to an extension of Sard’s Theorem by (Bhattacharya and Patrangenaru, 2003, p.12) for a closed manifold, \( \Phi \) is univalent up to a set of Lebesgue measure zero. Then the set of extrinsic means is given by the set of images \( \Phi(E(Y)) \) where \( Y \) denotes \( X \) viewed as taking values in \( \mathbb{R}^D \) (cf. Bhattacharya and Patrangenaru (2003)).

Residual means. In this context, setting \( \rho^{(r)}(p, p') = \|d\Phi_p(p - p')\| \) \( (p, p' \in M) \) with the derivative \( d\Phi_p \) at \( p' \) yielding the orthogonal projection to the embedded tangent space \( T_p \mathbb{R}^D \to T_p M \subset T_p \mathbb{R}^D \), call the corresponding mean sets \( E^{(\rho^{(r)})}(X) \) and \( E^{(\rho^{(r)})}(\omega) \), the sets of residual population means and residual sample means, respectively. For two-spheres, \( \rho^{(r)}(p, p') \) has been studied under the name of crude residuals by Jupp (1988). On unit-spheres

\[
\rho^{(r)}(p, p') = \|p - \langle p, p' \rangle p'\| = \sqrt{1 - \langle p, p' \rangle^2} = \rho^{(r)}(p', p)
\]

is a quasi-metric (symmetric, vanishing on the diagonal \( p = p' \) and satisfying the triangle inequality). On general manifolds, however, the residual distance \( \rho^{(r)} \) may be neither symmetric nor satisfying the triangle inequality.

Obviously, for \( X \) uniformly distributed on a sphere, the entire sphere is identical with the set of intrinsic, extrinsic and residual means: non-unique intrinsic and extrinsic means may depend counterintuitively on the dimension of the ambient space. Here is a simple illustration.

Proposition 3.2. Suppose that \( X \) is a random point on a unit sphere \( S^{D-1} \) that is uniformly distributed on a unit subsphere \( S \). Then

(i) every point on \( S^{D-1} \) is an extrinsic mean and,

(ii) if \( S \) is a proper subsphere then the set of intrinsic means is equal to the unit subsphere \( S' \) orthogonal to \( S \).
Proof. The first assertion is a consequence of \( \rho(e)(x,y)^2 + \rho(e)(x,-y)^2 = 4 \) for every \( x, y \in S^{D-1} \). The second assertion follows from
\[
\rho(i)(x,y)^2 + \rho(i)(x,-y)^2 = \rho(i)(x,y)^2 + (\pi - \rho(i)(x,y))^2 \geq \frac{\pi^2}{2}
\]
for the intrinsic distance \( \rho(i)(x,y) = 2 \arcsin(\|x-y\|/2) \) with equality if and only if \( x \) is orthogonal to \( y \).

\[\square\]

Proposition 3.3. If a random point \( X \) on a unit sphere is a.s. contained in a unit subsphere \( S \) then \( S \) contains every residual mean as well as every unique intrinsic or extrinsic mean.

Proof. Suppose that \( x = v + \nu \) is a mean of \( X \) with \( v/\|v\| \in S \) and \( \nu \in S^{D-1} \) normal to \( S \). Since \( 1 - \langle X, v + \nu \rangle^2 = 1 - \langle X, v \rangle^2 \geq 1 - \langle X, v \rangle^2 / \|v\|^2 \) a.s. with equality if and only if \( \nu = 0 \), the assertion for residual means follows at once from (2). For intrinsic and extrinsic means we argue with \( \|X - (v + \nu)\| = \|X - (v - \nu)\| \) a.s. yielding \( \nu = 0 \) in case of uniqueness.

\[\square\]

Let us now incorporate more of the structure common to shape spaces. The following definition is due to [Kendall et al., 1999, p. 249]. We additionally require that the group acting be compact in order to ensure that the quotient be Hausdorff. More generally, one could assume a non-compact group acting properly, cf. [Palais, 1961].

Definition 3.4. A complete connected finite-dimensional Riemannian manifold \( M \) with geodesic distance \( d_M \) on which a compact Lie group \( G \) acts isometrically from the left is called a \textit{pre-shape space}. Moreover the canonical quotient
\[
\pi : M \to Q := M/G = \{[p] : p \in M\}
\]
with the orbit \([p] = \{gp : g \in G\}\), is called a shape space.

As a consequence of the isometric action we have that \( d_M(gp, p') = d(p, g^{-1}p') \) for all \( p, p' \in M, g \in G \). For \( p, p' \in M \) we say that \( p \) is in \textit{optimal position} to \( p' \) if \( d_M(p, p') = \min_{g \in G} d_M(gp, p') \), the minimum is attained since \( G \) is compact. As is well known (e.g. [Bredon, 1972, p. 179]) there is an open and dense submanifold \( M^* \) of \( M \) such that the canonical quotient \( Q^* = M^*/G \) restricted to \( M^* \) carries a natural manifold structure also being open and dense in \( Q \). Elements in \( M^* \) and \( Q^* \), respectively, are called \textit{regular}, the complementary elements are \textit{singular}; \( Q^* \) is the \textit{manifold part} of \( Q \).

Intrinsic means on shape spaces. The canonical quotient distance
\[
d_Q([p], [p']) := \min_{g \in G} d_M(gp, p') = \min_{g, h \in G} d_M(gp, hp')
\]
is called \textit{intrinsic distance} and the corresponding \( d_Q \)-Fréchet mean sets are called \textit{intrinsic means}. Note that the intrinsic distance on \( Q^* \) is equal to the canonical geodesic distance.
Ziezold and Procrustean means. Now, assume that we have an embedding with orthogonal projection $\Phi : \mathbb{R}^D \to M \subset \mathbb{R}^D$ as above. If the action of $G$ is isometric w.r.t. the extrinsic metric, i.e. if $\|gp - gp'\| = \|p - p'\|$ for all $p, p' \in M$ and $g \in G$ then call

$$\rho_Q^{(z)}([p], [p']) := \min_{g \in G} \|gp - p'\|$$
and

$$\rho_Q^{(p)}([p], [p']) := \min_{g \in G, \text{gp in opt. pos. to } p'} d\Phi_p(gp - p)$$

the Ziezold distance and the Procrustean distance on $Q$, respectively. Call the corresponding population and sample Fréchet $\rho_Q^{(z)}$-means, respectively, the sets of population and sample Ziezold means, respectively. Similarly, call the corresponding population and sample Fréchet $\rho_Q^{(p)}$-means, respectively, the sets of population and sample Procrustean means, respectively.

We say that optimal positioning is invariant if for all $p, p' \in M$ and $g^* \in G$,

$$d_M(g^*p, p') = \min_{g \in G} d_M(gp, p') \Leftrightarrow \|g^*p - p'\| = \min_{g \in G} \|gp - p'\|.$$

**Remark 3.5.** Indeed for $Q = \Sigma_m^{ck}, R\Sigma_m^{ck}$, optimal positioning is invariant (cf. [Kendall et al., 1993, p. 206]), Procrustean means coincide with means of general Procrustes analysis introduced by [Gower, 1973] and Ziezold means coincide with means as introduced by [Ziezold, 1994] for $\Sigma_2^k$. Moreover for $\Sigma_2^k$, Procrustean means agree with extrinsic means w.r.t. the Veronese-Whitney embedding, cf. [Bhattacharya and Patrangenaru, 2003] and Section 5.

Procrustean means on $\Sigma_m^{ck}$ are also called full Procrustes means in the literature to distinguish them from partial Procrustes means on the size-and-shape spaces not further discussed here (e.g. [Dryden and Mardia, 1998]). We only note that partial Procrustes means are identical to the respective intrinsic, Procrustean and Ziezold means which on size-and-shape spaces, all agree with one another.

4 Horizontal Lifting and Manifold Stability

In this section we derive a measurable horizontal lifting and the stability theorem underlying Theorem 2.2. To this end we first recall how a shape space is made up from manifold strata of varying dimensions. Unless otherwise referenced, we use basic terminology that can be found in any standard textbook on differential geometry, e.g. [Kobayashi and Nomizu, 1963, 1969]. For the results derived here we assume that the shape space is a quotient modulo a compact group. We note that these results remain valid in the more general case of a non-compact group acting properly, cf. [Palais, 1961].
4.1 Preliminaries

Assume that $Q = M/G$ is a shape space as in Definition 3.4. $T_p M$ is the tangent space of $M$ at $p \in M$ and $\exp_p$ denotes the Riemannian exponential at $p$. Recall that on a Riemannian manifold the cut locus $C(p)$ of $p$ comprises all points $q$ such that the extension of a length minimizing geodesic joining $p$ with $q$ is no longer minimizing beyond $q$. In consequence, on a complete and connected manifold $M$ we have for every $p' \in M$ that there is $v' \in T_{p'} M$ such that $p' = \exp_{p'} v'$ while $v' = \exp_{p^{-1}} p'$ of minimal modulus is uniquely determined as long as $p' \in M \setminus C(p)$. It is well known that the cut locus has measure zero in the sense that its image in any local chart has Lebesgue measure zero. From now on we call the cut locus the manifold cut locus of the manifold part $M$ and connected manifold $p$ determined as long as $p$ is of different. In particular, quotient cut loci are void in the special case of Kendall’s shape spaces.

**Lemma 4.1.** $C(q) \neq \emptyset$ for every $q \in \Sigma^K$ while $C^{\text{quot}}(q) = \emptyset$ for all $q \in \Sigma^K$. Similarly $C^{\text{quot}}(q) = \emptyset$ for all $q \in R^{\Sigma^K}$.

**Proof.** The first assertion follows from the fact that $\Sigma^K$ is a compact manifold. For the second assertion consider $[p] \in \Sigma^K$. Since $C(p) = \{ -p \}$ for $p \in S^k$ and $[p] = [-p]$ for even $m$ as well as for odd $m$ if $p$ is not regular, and, since $p$, $-p$ are not in optimal position for odd $m$ if $p$ is regular, we have that $C^{\text{quot}}([p]) = \emptyset$. The third assertion follows from the fact that $[p] = [-p]$ for all $[p] \in R^{\Sigma^K}$. $\square$

Next we collect consequences of the isometric Lie group action, see [Bredon 1972].

(A) With the *isotropy group* $I_p = \{ g \in G : gp = p \}$ for $p \in M$, every orbit carries the natural structure of a coset space $[p] \cong G/I_p$. Moreover, $p' \in M$ is of *orbit type* $(G/I_p)$ if $I_{p'} = g I_p g^{-1} = I_g p$ for a suitable $g \in G$. If $I_p \subset I_g p'$ for suitable $g \in G$ then $p'$ is of *lower orbit type* than $p$ and $p$ is of *higher orbit type* than $p'$.

(B) The pre-shapes of equal orbit type $M^{(I_p)} := \{ p' \in M : p' \text{ is of orbit type } (G/I_p) \}$ and the corresponding shapes $Q^{(I_p)} := \{ [p'] : p' \in M^{(I_p)} \}$ are manifolds in $M$ and $Q$, respectively. Moreover, for $q \in Q$ denote by $Q^{(q)}$ the shapes of higher orbit type.

(C) The orthogonal complement $H_p M$ in $T_p M$ of the tangent space $T_p[p]$ along the orbit is called the *horizontal space*: $T_p M = T_p[p] \oplus H_p M$. 

10
The Slice Theorem states that every $p \in M$ has a tubular neighborhood $[p] \subset U \subset M$ such that with a suitable subset $D \subset H_p M$ the twisted product $\exp_p D \times I_p G$ is diffeomorphic with $U$. Here, the twisted product is the natural topological quotient of the product space $\exp_p D \times G$ modulo the equivalence

$$(\exp_p v, g) \sim_{I_p} (\exp_p v', g') \iff \exists h \in I_p \text{ such that } v' = dhv, \ g' = gh^{-1}.$$ 

We then say that the tubular neighborhood $U$ admits a slice $\exp_p D$ via $U \cong \exp_p D \times I_p G$.

Every $p \in M$ has a tubular neighborhood $U$ of $p$ that admits a slice $\exp_p D$ such that every $p' \in \exp_p D$ is in optimal position to $p$. Moreover, for any tubular neighborhood $U$ admitting a slice $\exp_p D$, all points $p' \in U$ are of orbit type higher than or equal to the orbit type of $p$ and only finitely many orbit types occur in $U$. If $p$ is regular, i.e. of maximal orbit type, then the product is trivial: $\exp_p D \times I_p G \cong \exp_p D \times G/I_p$.

Finally let us extend the following uniqueness property for the intrinsic distance to the Ziezold distance. The differential of the mapping $f^\prime_{\text{in}} : M \setminus C(p') \to [0, \infty)$ defined by $f^\prime_{\text{in}}(p) = d_M(p, \exp_p p')^2$ is given by $df^\prime_{\text{in}}(p) = -2v$ with $v = \exp^{-1}_p p'$ (cf. [Kobayashi and Nomizu, 1969, p. 110], [Karcher, 1977]). Hence, we have for $p_1, p_2 \in M \setminus C(p)$ that

$$df^\prime_{\text{in}}(p_1) = df^\prime_{\text{in}}(p_2) \iff p_1 = p_2.$$ 

(4)

In view of the extrinsic distance let $f^\prime_{\text{ext}} : M \setminus C(p') \to [0, \infty)$ be defined by $f^\prime_{\text{ext}}(p) = \|p - p\|_p^2 = \|p - \exp_p(\exp^{-1}_p p')\|^2$. Mimicking (4) introduce the following condition

$$df^\prime_{\text{ext}}(p_1) = df^\prime_{\text{ext}}(p_2) \iff p_1 = p_2$$

(5)

for $p_1, p_2 \in M \setminus C(p)$.

Remark 4.2. (4) is valid on closed half spheres since on the unit sphere

$$df^\prime_{\text{ext}}(p) = -2 \frac{v}{\|v\|} \sin(\|v\|) \text{ with } v = \exp^{-1}_p p'.$$

4.2 A Measurable Horizontal Lift

In order to establish the stability of means in Theorem 4.7 in the following Section 4.3, here we lift a random shape $X$ from $Q$ horizontally to a random pre-shape $Y$ on $M$. In order to do so we need to guarantee the measurability of the horizontal lift in Theorem 4.4 below, the proof of which can be found in the appendix.

Before continuing, let us consider a simple example for illustration. Suppose that $G = S^1 \subset \mathbb{C}$ acts on $M = \mathbb{C}$ by complex scalar multiplication. Then
With a measurable horizontal lift $L^p$ to $p$.

Theorem 4.4. Let $\rho$ be able horizontal lift $L^p$ of a measurable subset $R$ of $M/G$ in optimal position to $p \in M$ if

1. the canonical projection $L \to R \subset M/G$ is surjective,
2. every $p' \in L$ is in optimal position to $p \in L$,
3. every orbit $[p']$ of $p' \in L$ meets $L$ once.

Theorem 4.5. Assume that $X$ is a random shape on $Q$ and that there are $p \in M$ and $A \subset Q$ countable such that $X$ is supported by $(Q^{(p)} \cup A) \setminus C^{\text{quot}}([p])$. With a measurable horizontal lift $L$ of $(Q^{(p)} \cup A) \setminus C^{\text{quot}}([p])$ in optimal position to $p$ define the random element $Y$ on $L \subset M$ by $\pi \circ Y = X$.

(i) If $[p]$ is an intrinsic mean of $X$ on $Q$, then $p$ is an intrinsic mean of $Y$ on $M$ and
\[ \mathbb{E}(\exp_p^{-1} Y) = 0. \]

(ii) If $[p]$ is a Ziezold mean of $X$ on $Q$ and optimal positioning is invariant, then $p$ is an extrinsic mean of $Y$ on $M$ and
\[ \mathbb{E}(d_{\text{ext}}^Y(p)) = 0. \]

(iii) If $[p]$ is a Procrustean mean of $X$ on $Q$ and optimal positioning is invariant, then $p$ is a residual mean of $Y$ on $M$.

Proof. Suppose that $[p]$ is an intrinsic mean of $X$. If $p$ would not be an intrinsic mean of $Y$, there would some $M \ni p' \neq p$ leading to the contradiction
\[ \mathbb{E}(d_Q([p'], X)^2) = \mathbb{E}(d_M(p', Y)^2) < \mathbb{E}(d_M(p, Y)^2) = \mathbb{E}(d_Q([p], X)^2). \]

Hence, $p$ is an intrinsic mean of $Y$. Replacing $d_Q$ by $\rho_Q^{(p)}$ and $d_M$ by the Euclidean distance gives the assertion for Ziezold and extrinsic means, respectively; and, using the Procrustean distance $\rho_Q^{(p)}$ on $Q$ as well as the residual distance $\rho_M^{(p)}$ on $M$ gives the assertion for Procrustean and residual means, respectively.

For intrinsic means $p \in M$, the necessary condition $\mathbb{E}(\exp_p^{-1} Y) = 0$ is developed in [Kobayashi and Nomizu, 1969, p. 110], cf. also [Karcher, 1977].
(Kendall, 1990, p. 395) which yields the asserted equality in (i). By definition, the analog condition for an extrinsic mean $p \in M$ is $E(df^X_{ext}(p)) = 0$ which is the asserted equality in (ii) completing the proof. 

**Remark 4.6.** Since the maximal intrinsic distance on $\Sigma^k_m$ and $R\Sigma^k_m$ is

$$\pi 2 = \max_{x,y \in S^m_k} \min_{g \in SO(m)} \arccos \left( \text{tr}(gxy^T) \right) = \max_{x,y \in S^m_k} \min_{g \in O(m)} \arccos \left( \text{tr}(gxy^T) \right),$$

taking into account Remark 4.2, condition (5) is satisfied for any horizontal lift in optimal position.

### 4.3 Manifold Stability

The proof of the following central theorem is deferred to the appendix.

**Theorem 4.7.** Assume that $X$ is a random shape on $Q$, $p \in M$ and that $A \subset Q$ is countable such that $X$ is supported by $(Q[p] \cup A) \setminus C^\text{quot}([p])$ and let $p' \in [p] \in Q([p])$. If $P\{X \in Q[p']\} \neq 0$ and if either $[p]$ is

(i) an intrinsic mean of $X$ or

(ii) a Ziezold mean of $X$ while optimal positioning is invariant and (5) is valid,

then $p'$ is of lower orbit type than $p$.

We have at once the following Corollary.

**Corollary 4.8** (Manifold Stability Theorem). Suppose that $X$ is a random shape on $Q$ that is supported by $Q \setminus C^\text{quot}([p])$ for some $[p] \in Q$ assuming the manifold part $Q^*$ with non-zero probability and having at most countably many point masses on the singular part. Then $[p]$ is regular if it is an intrinsic mean of $X$, or if it is a Ziezold mean, optimal positioning is invariant and (5) is valid.

Since $Q \setminus Q(q)$ is a null set in $Q$ for every $q \in Q$ (cf. Bredon [1972, p. 184]) and so is $C^\text{quot}(q)$ – by (5) it is contained in the projection of a null set – we have the following practical application.

**Corollary 4.9.** Suppose that a random shape on $Q$ is absolutely continuously distributed w.r.t. the projection of the Riemannian volume on $M$. Then intrinsic and Ziezold population means are regular; the latter if optimal positioning is invariant and (5) is valid. And, intrinsic and Ziezold sample means are a.s. regular.

### 4.4 An Example for Non-Stability of Procrustean Means

Consider a random configuration $Z \in F_3^4$ assuming the collinear quadrangle $q_1$ with probability 2/3 and the planar quadrangle $q_2$ with probability 1/3 where

$$q_1 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad q_2 = \begin{pmatrix} 1 & 1 & -2 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{3}{\sqrt{2}} \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$
Corresponding pre-shapes in optimal position w.r.t. the action of \( SO(3) \) and \( O(3) \) are given by

\[
p_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad p_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.
\]

Note that \([p_2]\) has regular shape in \((\Sigma_3^4)^*\). The full Procrustes mean of \([Z] \in \Sigma_3^4\) is easily computed to have the singular shape \([p_1] \in \Sigma_3^4 \setminus (\Sigma_3^4)^*\), see Figure 2 as well as Examples 6.5 and Section 7.2. Cf. also Remark 2.3.

## 5 Extrinsic Means for Kendall’s (Reflection) Shape Spaces

Let us recall the well known Veronese-Whitney embedding for Kendall’s planar shape spaces \( \Sigma_2^k \). Identify \( F_2^k \) with \( \mathbb{C}^{k-1} \setminus \{0\} \) such that every landmark column corresponds to a complex number. This means in particular that \( z \in \mathbb{C}^{k-1} \) is a complex row(!)-vector. With the Hermitian conjugate \( a^* = (\overline{a_{kj}}) \) of a complex matrix \( a = (a_{jk}) \) the pre-shape sphere \( S_2^k \) is identified with \( \{ z \in \mathbb{C}^{k-1} : zz^* = 1 \} \) on which \( SO(2) \) identified with \( S^1 = \{ \lambda \in \mathbb{C} : |\lambda| = 1 \} \) acts by complex scalar multiplication. Then the well known Hopf-Fibration mapping to complex projective space gives \( \Sigma_2^k = S_2^k / S^1 = \mathbb{C}P^{k-2} \). Moreover, denoting with \( M(k-1, k-1, \mathbb{C}) \) all complex \((k-1) \times (k-1)\) matrices, the Veronese-Whitney embedding is given by

\[
S_2^k / S^1 \rightarrow \{ a \in M(k-1, k-1, \mathbb{C}) : a^* = a \}, \quad [z] \mapsto z^*z.
\]

**Remark 5.1.** The Procrustean metric of \( \Sigma_2^k \) is isometric with the Euclidean metric of \( M(k-1, k-1, \mathbb{C}) \) since we have \( \langle z, w \rangle = \text{Re}(zw^*) \) for \( z, w \in S_2^k \) and hence, \( d_{\Sigma_2^k}^2([z], [w]) = 1 - w^*z^*w = ||w^*w - z^*z||/\sqrt{2} \).

The idea of the Veronese-Whitney embedding can be carried to the general case of shapes of arbitrary dimension \( m \geq 2 \). Even though the embedding given below is apt only for reflection shape space it can be applied to practical situations in similarity shape analysis whenever the geometrical objects considered have a common orientation. As above, the number \( k \) of landmarks is essential and will be considered fixed throughout this section; the dimension \( 1 \leq m < k \), however, is lost in the embedding and needs to be retrieved by projection. To this end recall the embedding of \( S_j^k \) in \( S_m^k \) \((1 \leq j \leq m) \) in \( \mathbb{U} \) which gives rise to a canonical embedding of \( R\Sigma_j^m \) in \( R\Sigma_j^k \). Moreover, consider the strata

\[
(R\Sigma_m^k)^j := \{ [x] \in R\Sigma_m^k : \text{rank}(x) = j \}, \quad (\Sigma_m^k)^j := \{ [x] \in \Sigma_m^k : \text{rank}(x) = j \}
\]

for \( j = 1, \ldots, m \), each of which carries a canonical manifold structure; due to the above embedding, \((R\Sigma_m^k)^j\) will be identified with \((R\Sigma_j^k)^j\) such that

\[
R\Sigma_m^k = \bigcup_{j=1}^m (R\Sigma_j^k)^j,
\]

14
and \((\Sigma_m^k)^j\) with \((\Sigma_m^k)^j\) in case of \(j < m\). At this point we note that \(SO(m)\) is connected, while \(O(m)\) is not; and the consequences for the respective manifold parts, i.e. points of maximal orbit type:

\[
(\Sigma_m^k)^* = (\Sigma_m^k)^{m-1} \cup (\Sigma_m^k)^m, \quad (R\Sigma_m^k)^* = (R\Sigma_m^k)^m. \quad (6)
\]

Similarly, we have a stratification

\[
P := \left\{ a \in M(k-1, k-1) : a = a^T \geq 0, \text{tr}(a) = 1 \right\} = \bigcup_{j=1}^{k-1} P^j
\]

of a compact flat convex space \(P\) with non-flat manifolds \(P^j := \{ a \in P : \text{rank}(a) = j \} \) \((j = 1, \ldots, k-1)\), all embedded in \(M(k-1, k-1)\). The Schoenberg map \(s : R\Sigma_m^k \to P\) is then defined on each stratum by

\[
s_{(R\Sigma_m^k)^j} := s^j : (R\Sigma_m^k)^j \to P^j, \quad [x] \mapsto x^T x.
\]

For \(x \in S_j^k\) recall the tangent space decomposition \(T_x S_j^k = T_x[x] \oplus H_x S_j^k\) into the vertical tangent space along the orbit \([x]\) and its orthogonal complement the horizontal tangent space. For \(x \in (S_j^k)^j\) identify canonically (cf. [Kendall et al., 1999, p. 109]):

\[
T_{[x]}(R\Sigma_j^k)^j \cong H_x S_j^k = \{ w \in M(j, k-1) : \text{tr}(wx^T) = 0, wx^T = xw^T \}.
\]

Then the assertion of the following Theorem condenses results of Bandulasiri and Patrangenaru [2005], cf. also Dryden et al. [2008].

**Theorem 5.2.** Each \(s^j\) is a diffeomorphism with inverse \((s^j)^{-1}(a) = \left[ (\sqrt{\lambda u^T})^j \right]\) where \(a = u\lambda u^T\) with \(u \in O(k-1)\), \(\lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)\), and \(0 = \lambda_{j+1} = \ldots = \lambda_{k-1}\) in case of \(j < k - 1\). Here, \((a)^j_1\) denotes the matrix obtained from taking only the first \(j\) rows from \(a\). For \(x \in S_j^k\) and \(w \in H_x S_j^k \cong T_{[x]}(R\Sigma_j^k)^j\) the derivative is given by

\[
d(s^j)^j w = x^T w + w^T x.
\]

**Remark 5.3.** In contrast to the Veronese-Whitney embedding, the Schoenberg embedding is not isometric as the example of

\[
x = \begin{pmatrix}
\cos \phi & 0 \\
0 & \sin \phi
\end{pmatrix}, \quad w_1 = \begin{pmatrix}
\sin \phi & 0 \\
0 & -\cos \phi
\end{pmatrix}, \quad w_2 = \begin{pmatrix}
0 & \cos \phi \\
\sin \phi & 0
\end{pmatrix},
\]

teaches: \(\|x^T w_1 + w_1^T x\| = \sqrt{2} |\cos \phi \sin \phi|\), \(\|x^T w_2 + w_2^T x\| = \sqrt{2}\).

Since \(P\) is bounded, convex and Euclidean, the classical expectation \(E(X^T X) \in P^j\) for some \(1 \leq j \leq k - 1\) of the Schoenberg image \(X^T X\) of an arbitrary random reflection shape \([X] \in R\Sigma_m^k\) is well defined. Then we have at once the following relation between the rank of the Euclidean mean and increasing sample size.
Theorem 5.4. Suppose that a random reflection shape \([X] \in R\Sigma^k_m\) is distributed absolutely continuous w.r.t. the projection of the spherical volume on \(S^k_m\). Then
\[
E(X^T X) \in P^{k-1} \quad \text{and} \quad \frac{1}{n} \sum_{i=1}^{n} X_i^T X_i \in P^{\min(nm,k-1)} \quad \text{a.s.,}
\]
for every i.i.d. sample \(X_1, \ldots, X_n \sim X\).

Hence, in statistical settings involving a higher number of landmarks, a sufficiently well behaved projection of a high rank Euclidean mean onto lower rank \(P^r \cong (\Sigma^k_r)^r\), usually \(m = r\), is to be employed, giving at once a mean shape satisfying strong consistency and a CLT. Here, unlike to intrinsic or Procrustes analysis, the dimension \(r\) chosen is crucial for the dimensionality of the mean obtained.

The orthogonal projection
\[
\phi^r : \bigcup_{i=1}^{k-1} P^i \rightarrow P^r, \quad a \mapsto \arg\min_{b \in P^r} \text{tr} \left( (a - b)^2 \right)
\]
giving the set of extrinsic Schoenberg means has been computed by Bhattacharya (2008):

Theorem 5.5. For \(1 \leq r \leq k - 1\), \(a = u\lambda u^T \in P\) with \(u \in O(k - 1)\), \(\lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)\), \(\lambda_1 \geq \ldots \geq \lambda_{k-1}\) and \(\lambda_r > 0\) the orthogonal projection onto \(P^r\) is given by \(\phi^r(a) = u\mu u^T\) with \(\mu = \text{diag}(\mu_1, \ldots, \mu_r, 0, \ldots, 0)\),
\[
\mu_i = \lambda_i + \frac{1}{r} - \frac{\lambda_r}{r} \quad (i = 1, \ldots, r)
\]
and \(\lambda_r = \frac{1}{r} \sum_{i=1}^{r} \lambda_i \leq \frac{1}{r}\) which is uniquely determined if and only if \(\lambda_r > \lambda_{r+1}\).

With the notation of Theorem 5.5, a non-orthogonal central projection \(\psi^r(a) = uu^T\) equally well and uniquely determined has been proposed by Dryden et al. (2008) with
\[
\nu = \text{diag}(\nu_1, \ldots, \nu_r, 0, \ldots, 0), \quad \nu_i = \frac{\lambda_i}{r\lambda_r} \quad (i = 1, \ldots, r).
\]

Orthogonal and central projection are depicted in Figure 1.

6 Local Effects of Curvature

In this section we assume that a manifold stratum \(M\) supporting a random element \(X\) is isometrically embedded in a Euclidean space \(\mathbb{R}^D\) of dimension \(D > 0\). With the orthogonal projection \(\Phi : \mathbb{R}^D \rightarrow M\) from Section 3 and the Riemannian exponential \(\exp_p\) of \(M\) at \(p\) we have the
\[
\text{intrinsic tangent space coordinate} = \exp_p^{-1} X \quad \text{and} \quad \text{residual tangent space coordinate} = d\Phi_p(X - p),
\]
respectively, of \(X\) at \(p\), if existent.
Figure 1: Projections (if existent) of two points (crosses) in the $\lambda$-plane to the open line segment $\Lambda = \{(\lambda_1, \lambda_2) : \lambda_1 + \lambda_2 = 1, \lambda_1, \lambda_2 > 0\}$. The dotted line gives the central projections (denoted by stars) which is well defined for all symmetric, positive definite matrices (corresponding to the first open quadrant), the dashed line gives the orthogonal projection (circle) which is well defined in the triangle below $\Lambda$ (corresponding to $P$) and above $\Lambda$ in an open strip. In particular it exists not for the right point.

6.1 Finite Power of Tests and Tangent Space Coordinates

With the above setup, assume that $\mu \in M$ is a unique mean of $X$. Moreover, we assume that $M$ is curved near $\mu$, i.e. that there is $c \in \mathbb{R}^D$, the center of the osculatory circle touching the geodesic segment in $M$ from $X$ to $\mu$ at $\mu$ with radius $r$. If $X_r$ is the orthogonal projection of $X$ to that circle, then $X = X_r + O(\|X - \mu\|^3)$. Moreover, with

$$\cos \alpha = \left\langle \frac{X - c}{\|X - c\|}, \frac{\mu - c}{r} \right\rangle = \frac{1}{r^2} (X_r - c, \mu - c) + O(\|X - \mu\|^3)$$

we have the residual tangent space coordinate

$$v = X - c - \frac{\mu - c}{r} \|X - c\| \cos \alpha = X_r - c - (\mu - c) \cos \alpha + O(\|X - \mu\|^3)$$

having squared length $\|v\|^2 = r^2 \sin^2 \alpha + O(\|X - \mu\|^3)$. By isometry of the embedding, the intrinsic tangent space coordinate is given by

$$\exp^{-1}_\mu X = \frac{r \alpha}{\|v\|} v + O(\|X - \mu\|^3).$$

With the component

$$\nu = \mu - c - \|X - c\| \frac{\mu - c}{r} \cos \alpha = (\mu - c)(1 - \cos \alpha) + O(\|X - \mu\|^3)$$

of $X$ normal to the above mentioned geodesic segment of squared length $\|\nu\|^2 = r^2 (1 - \cos \alpha)^2 + O(\|X - \mu\|^3)$, we obtain $\|\exp^{-1}_\mu X\|^2 = \|v\|^2 + \|\nu\|^2 + O(\|X - \mu\|^3)$, since

$$(1 - \cos \alpha)^2 + \sin^2 \alpha = 2(1 - \cos \alpha) = \alpha^2 + 2 \frac{\alpha^4}{4!} + \cdots$$

and $\alpha = O(\|X - \mu\|)$. In consequence we have
Remark 6.1. In approximation, the variation of intrinsic tangent space coordinates is the sum of the variation $\|v\|^2$ of residual tangent space coordinates and the variation normal to it. In particular, for spheres

$$\|\exp_p^{-1}X\|^2 \geq \|v\|^2 + \|\nu\|^2.$$  

Since the variation in normal space is irrelevant for a two-sample test for equality of means, say, a higher power for tests based on intrinsic means can be expected when solely residual tangent space coordinates obtained from an isometric embedding are used rather than intrinsic tangent space coordinates.

Note that the natural tangent space coordinates for Ziezold means are residual.

A simulated classification example in Section 7 illustrates this effect.

6.2 The 1 : 3 - Property for Spherical and Kendall Shape Means

In this section $M = S^{D-1} \subset \mathbb{R}^D$ is the $(D-1)$-dimensional unit-hypersphere embedded isometrically in Euclidean $D$-dimensional space. The orthogonal projection $\Phi : \mathbb{R}^D \to S^{D-1} : p \to \frac{p}{\|p\|}$ is well defined except for the origin $p = 0$, and the normal space at $p \in S^{D-1}$ is spanned by $p$ itself. In consequence, a random point $X$ on $S^{D-1}$ has

$$d\Phi_p(X - p) = X - p \cos \alpha, \quad \exp_p^{-1}(X) = \begin{cases} \frac{\sin \alpha}{\sin \alpha} d\Phi_p(X - p) & \text{for } X \neq p \\ 0 & \text{for } X = p \end{cases}$$

as residual and intrinsic, resp., tangent space coordinate at $-X \neq p \in S^{D-1}$ where $\cos \alpha = \langle X, p \rangle$, $\alpha \in [0, \pi)$.

Theorem 6.2. If $X$ a.s. is contained in an open half sphere, it has a unique intrinsic mean which is assumed in the interior of that half sphere.

Proof. Below, we show that every intrinsic mean necessarily lies within the interior of the half sphere. Then, (Kendall 1990, Theorem 7.3) yields uniqueness. W.l.o.g. let $X = (\sin \phi, x_2, \ldots, x_n)$ such that $P\{\sin \phi \leq 0\} = 0 = 1 - P\{\sin \phi > 0\}$ and assume that $p = (\sin \psi, p_2, \ldots, p_n) \in S^{D-1}$ is an intrinsic mean, $-\pi/2 \leq \phi, \psi \leq \pi/2$. Moreover let $p' = (\sin(|\psi|), p_2, \ldots, p_n)$. Since

$$E \left( \|\exp_p^{-1}(X)\|^2 \right) = E \left( \arccos^2 \langle p, X \rangle \right)$$

$$= E \left( \arccos^2 \left( \sin \psi \sin \phi + \sum_{j=2}^{n} p_j x_j \right) \right)$$

$$\geq E \left( \|\exp_{p'}^{-1}(X)\|^2 \right)$$

18
with equality if and only if $\sin |\psi| = \sin \psi$, this can only happen for $\sin \psi \geq 0$.

Now, suppose that $p = (0, p_2, \ldots, p_n)$ is an intrinsic mean. For small deterministic $\psi \geq 0$ consider $p(\psi) = (\sin \psi, p_1 \cos \psi, \ldots, p_n \cos \psi)$. Then

$$
\mathbb{E} \left( \| \exp_{p(\psi)}^{-1}(X) \|^2 \right) = \mathbb{E} \left( \arccos^2 \left( \sin \psi \sin \phi + \cos \psi \sum_{j=2}^{n} p_j x_j \right) \right)
$$

$$
= \mathbb{E} \left( \| \exp_{p}^{-1}(X) \|^2 \right) - C_1 \psi + O(\psi^2)
$$

with $C_1 > 0$ since $\mathbb{P}\{\sin \phi > 0\} > 0$. In consequence, $p$ cannot be an intrinsic mean. Hence, we have shown that every intrinsic mean is contained in the interior of the half sphere.

Remark 6.3. For the special case of spheres, this is a simple proof for the general theorem recently established by Afsari (2010) which extends results of Karcher (1977); Kendall (1990) and Le (2001, 2004), stating that the intrinsic mean on a general manifold is unique if among others the support of the distribution is contained in a geodesic half ball.

The following theorem characterizes the three spherical means.

Theorem 6.4. Let $X$ be a random point on $S^{D-1}$. Then $x^{(e)} \in S^{D-1}$ is the unique extrinsic mean if and only if the Euclidean mean $E(X) = \int_{S^{D-1}} X dP_X$ is non-zero. In that case

$$
\lambda^{(e)} x^{(e)} = E(X)
$$

with $\lambda^{(e)} = \|E(X)\| > 0$. Moreover, there are suitable $\lambda^{(r)} > 0$ and $\lambda^{(i)} > 0$ such that every residual mean $x^{(r)} \in S^{D-1}$ satisfies

$$
\lambda^{(r)} x^{(r)} = E \left( \langle X, x^{(r)} \rangle X \right),
$$

and every intrinsic mean $x^{(i)} \in S^{D-1}$ satisfies

$$
\lambda^{(i)} x^{(i)} = E \left( \frac{\arccos \langle X, x^{(i)} \rangle}{\sqrt{1 - \langle X, x^{(i)} \rangle^2}} X \right).
$$

In the last case we additionally require that $\mathbb{E} \left( \frac{\arccos \langle X, x^{(i)} \rangle}{\sqrt{1 - \langle X, x^{(i)} \rangle^2}} \langle X, x^{(i)} \rangle \right) > 0$ which is in particular the case if $X$ is a.s. contained in an open half sphere.

Proof. The assertions for the extrinsic mean are well known from Hendriks et al. (1996). The second assertion for residual means follows from minimization of

$$
\int_{S^{D-1}} \| p - \langle p, x \rangle x \|^2 dP_X(p) = 1 - \int_{S^{D-1}} \langle p, x \rangle^2 dP_X(p)
$$

with respect to $x \in \mathbb{R}^D$ under the constraining condition $\|x\| = 1$. Using a Lagrange ansatz this leads to the necessary condition

$$
\int_{S^{D-1}} \langle p, x \rangle p dP_X(p) = \lambda x
$$
with a Lagrange multiplier $\lambda$ of value $E((X, x)^2)$ which is positive unless $X$ is supported by the hypersphere orthogonal to $x$. In that case, by Proposition 3.3, $x$ cannot be a residual mean of $X$, as every residual mean is as well contained in that hypersphere. Hence, we have $\lambda^{(r)} := \lambda > 0$.

The Lagrange method applied to

$$\int_{S^{D-1}} \|\exp^{-1}_x(p)\|^2 dP_X(p) = \int_{S^{D-1}} \arccos^2(\langle p, x \rangle) dP_X(p)$$

taking into account Theorem 6.2 insuring that $x^{(i)}$ is in the open half sphere that contains $X$ a.s., yields the third assertion on the intrinsic mean. $\square$

Recall that residual means are eigenvectors to the largest eigenvalue of the matrix $E(XX^T)$. As such, they rather reflect the mode than the classical mean of a distribution:

**Example 6.5.** Consider $\gamma \in (0, \pi)$ and a random variable $X$ on the unit circle \(\{e^{i\theta} : \theta \in [0, 2\pi]\}\) which takes the value 1 with probability $2/3$ and $e^{i\gamma}$ with probability $1/3$. Then, explicit computation gives the unique intrinsic and extrinsic mean as well as the two residual means

$$x^{(i)} = e^{i\gamma}, \quad x^{(e)} = e^{i\arctan \frac{\sin \gamma}{\sqrt{1 - \cos \gamma}}}, \quad x^{(r)} = \pm e^{i\arctan \frac{\sin(2\gamma)}{\sqrt{1 - \cos(2\gamma)}}}.$$

Figure 2 shows the case $\gamma = \frac{\pi}{2}$.

In contrast to Figure 2 one may assume in many practical applications that the mutual distances of the unique intrinsic mean $x^{(i)}$, the unique extrinsic mean $x^{(e)}$ and the unique residual mean $x^{(r)}$ closer to $x^{(e)}$ are rather small, namely of the same order as the squared proximity of the modulus $\|E(X)\|$ of the Euclidean mean to 1, cf. Table 2. We will use the following condition

$$\|x^{(e)} - x^{(r)}\|, \quad \|x^{(e)} - x^{(i)}\| = O((1 - \|E(X)\|)^2) \quad (7)$$

with the concentration parameter $1 - \|E(X)\|$.

**Corollary 6.6.** Under condition (7), if all three means are unique, then the great circular segment between the residual mean $x^{(r)}$ closer to the extrinsic
mean $x^{(r)}$ and the intrinsic mean $x^{(i)}$ is divided by the extrinsic mean in approximation by the ratio $1:3$:

$$x^{(r)} = \frac{\|E(X)\|}{\lambda^{(r)}} \left( x^{(e)} - \frac{E((X - x^{(e)}, X) X)}{\|E(X)\|} + O((1 - \|E(X)\|)^2) \right)$$

$$x^{(i)} = \frac{\|E(X)\|}{\lambda^{(i)}} \left( x^{(e)} + \frac{1}{3} \frac{E((X - x^{(e)}, X) X)}{\|E(X)\|} + O((1 - \|E(X)\|)^2) \right)$$

with $\lambda^{(i)}$ and $\lambda^{(r)}$ from Theorem 6.4.

Proof. For any $x,p \in S^{d-1}$ decompose $p - x = p - \langle x, p \rangle x - z(x, p)$ with $z(x, p) = 1 - \langle x, p \rangle$, the length of the part of $p$ normal to the tangent space at $x$. Note that $E(z(x, X)) = 1 - \|E(X)\|$. Now, under condition (7), verify the first assertion using Theorem 6.4:

$$x^{(r)} = \frac{1}{\lambda^{(r)}} \left( E(X) - E(z(x^{(r)}, X) X) \right).$$

On the other hand since

$$\arccos(1 - z) \sqrt{1 - (1 - z)^2} = 1 + \frac{1}{3} z + \frac{2}{15} z^2 + \ldots$$

we obtain with the same argument the second assertion

$$x^{(i)} = \frac{1}{\lambda^{(i)}} E \left( \frac{\arccos(x^{(e)}, X)}{\sqrt{1 - (1 - x^{(e)} X)^2}} X \right)$$

$$= \frac{1}{\lambda^{(i)}} \left( E(X) + \frac{1}{3} E \left( z(x^{(i)}, X) X \right) + \frac{2}{15} E \left( z(x^{(i)}, X) X \right) + \ldots \right)$$

$$= \frac{\|E(X)\|}{\lambda^{(i)}} \left( x^{(e)} + \frac{1}{3\|E(X)\|} E \left( z(x^{(e)}, X) X \right) + O((1 - \|E(X)\|)^2) \right).$$

\[\square\]

**Remark 6.7.** The tangent vector defining the great circle approximately connecting the three means is obtained from correcting with the expected normal component of any of the means. As numerical experiments show, this great circle is different from the first principal component geodesic as defined in Huckemann and Ziezold (2004).

Recall the following connection between top and quotient space means, cf. Theorem 4.3

**Remark 6.8.** Let $p \in S^k_m$ such that a random shape $X$ on $\Sigma^k_m$ is supported by $(\Sigma^k_m)^{(p)} \cup A$ with $A \subset \Sigma^k_m$ at most countable. By Lemma 4.2 and Theorem 4.3, $(\Sigma^k_m)^{(p)} \cup A$ admits a horizontal measurable lift $L \subset S^k_m$ in optimal position to $p \in S^k_m$. Define the random variable $Y$ on $L \subset S^k_m$ by $\pi \circ Y = X$. Then we have that
if \([p]\) is an intrinsic mean of \(X\) then \(p\) is an intrinsic mean of \(Y\),
if \([p]\) is a full Procrustean mean of \(X\) then \(p\) is a residual mean of \(Y\),
if \([p]\) is a Ziezold mean of \(X\) then \(p\) is an extrinsic mean of \(Y\).

In consequence, Corollary 6.6 extends at once to Kendall’s shape spaces. Generalized geodesics referred to below are an extension of the concept of geodesics to non-manifold shape spaces, cf. [Huckemann et al. (2010b)].

**Corollary 6.9.** Suppose that a random shape \(X\) on \(\Sigma^k_m\) with unique intrinsic mean \(\mu^{(i)}\), unique Ziezold mean \(\mu^{(z)}\) and unique Procrustean mean \(\mu^{(p)}\) is supported by 
\[ R = (\Sigma^k_m)(\mu^{(i)}) \cap (\Sigma^k_m)(\mu^{(z)}) \cap (\Sigma^k_m)(\mu^{(p)}). \]
If the means are sufficiently close to each other in the sense of
\[
d_{\Sigma^k_m} (\mu^{(z)} - \mu^{(p)}) , \quad d_{\Sigma^k_m} (\mu^{(z)} - \mu^{(i)}) = O((1 - \|E(Y)\|)^2)
\]
with the random pre-shape \(Y\) on a horizontal lift \(L\) of \(R\) defined by \(X = \pi \circ Y\), then the generalized geodesic segment between \(\mu^{(i)}\) and \(\mu^{(p)}\) is approximately divided by \(\mu^{(z)}\) by the ratio 1:3 with an error of order \(O((1 - \|E(Y)\|)^2)\).

**7 Examples: Exemplary Datasets and Simulations**

All of the results of this section are based on datasets and simulations, i.e., all means considered are sample means. An R-package for the computation of all means including the poplar leaves data can be found under [Huckemann (2010b)].

**7.1 The 1 : 3 property**

In the first example we illustrate Corollary 6.9 on the basis of four classical data sets:

**poplar leaves:** contains 104 quadrangular planar shapes extracted from poplar leaves in a joint collaboration with Institute for Forest Biometry and Informatics at the University of Göttingen, cf. [Huckemann (2010b); Huckemann et al. (2010a)].

**digits ’3’:** contains 30 planar shapes with 13 landmarks each, extracted from handwritten digits ’3’, cf. [Dryden and Mardia, 1998, p. 318].

**macaque skulls:** contains three-dimensional shapes with 7 landmarks each, of 18 macaque skulls, cf. [Dryden and Mardia, 1998, p. 16].

**iron age brooches:** contains 28 three-dimensional tetrahedral shapes of iron age brooches, cf. [Small, 1996, Section 3.5].

As clearly visible from Figure 3 and Table 2, the approximation of Corollary 6.9 for two- and three-dimensional shapes is highly accurate for data of little dispersion (the macaque skull data) and still fairly accurate for highly dispersed data (the digits ’3’ data).
means of 104 poplar leaf shapes
means of 30 digits ‘3’

means of 18 macaque skulls
means of 28 iron age brooches

Figure 3: Depicting shape means for four typical data sets: intrinsic (star), Ziezold (circle) and full Procrustes (diamond) projected to the tangent space at the intrinsic mean. The cross divides the generalized geodesic segment joining the intrinsic with the full Procrustes mean by the ratio 1 : 3.

Table 2: Mutual shape distances between intrinsic mean $\mu^{(i)}$, Ziezold mean $\mu^{(z)}$ and full Procrustes mean $\mu^{(p)}$ for various data sets. Last column: the concentration parameter from (7), cf. also Corollary 6.9.

| data set          | $d_{2,k} (\mu^{(i)}, \mu^{(z)})$ | $d_{2,k} (\mu^{(p)}, \mu^{(z)})$ | $d_{2,k} (\mu^{(p)}, \mu^{(i)})$ | $\parallel E(Y) \parallel^2$ |
|-------------------|---------------------------------|---------------------------------|---------------------------------|------------------------------|
| poplar leaves     | 0.66e-05                        | 1.83e-04                        | 2.44e-04                        | 5.24e-05                     |
| digits ‘3’        | 0.00154                         | 0.00452                         | 0.00605                         | 0.00155                      |
| macaque skulls    | 1.96e-05                        | 5.89e-05                        | 7.85e-05                        | 7.59e-06                     |
| iron age brooches | 0.000578                        | 0.001713                        | 0.002291                        | 0.000217                     |

7.2 “Partial Blindness” of full Procrustes and Schoenberg Means

In the second example we illustrate an effect of “blindness to data” of full Procrustes means and Schoenberg means. The former blindness is due to the affinity of the Procrustes mean to the mode in conjunction with curvature, the latter is due to non-isometry of the Schoenberg embedding. While the former effect occurs only for some highly dispersed data when the analog of condition (7) is violated, the latter effect is local in nature and may occur for concentrated data as well.
Reenacting the situation of Section 4.4 cf. also Example 6.5 and Figure 2, the shapes of the triangles $q_1$ and $q_2$ in Figure 4 are almost maximally remote. Since the mode $q_1$ is assumed twice and $q_2$ only once, the full Procrustes mean is nearly blind to $q_2$.

Even though Schoenberg means have been introduced to tackle 3D shapes, the effect of “blindness” can be well illustrated already for 2D. To this end consider $x = x(\phi)$, $w_1 = w_1(\phi)$ and $w_2 = w_2(\phi)$ as introduced in Remark 5.3. Along the horizontal geodesic through $x$ with initial velocity $w_2$ we pick two points $q_1 = x \cos \beta + w_2 \sin \beta$ and $q_2 = x \cos \beta - w_2 \sin \beta$. On the orthogonal horizontal geodesic through $x$ with initial velocity $w_1$ pick $q = x \cos \beta' + w_1 \sin \beta'$. Recall from Remark 5.3 that along that geodesic the derivative of the Schoenberg embedding can be made arbitrarily small for $\phi$ near 0. Indeed, Figure 5 illustrates
that in contrast to the intrinsic mean, the Schoenberg mean is “blind” to the strong collinearity of \( q_1 \) and \( q_2 \).

### 7.3 Discrimination Power

In the ultimate example we illustrate the consequences of the choice of tangent space coordinates and the effect of the tendency of the Schoenberg mean to increase dimension by a classification simulation. To this end we apply a Hotelling \( T^2 \)-test to discriminate the shapes of 10 noisy samples of regular unit cubes from the shapes of 10 noisy samples of pyramids with top section chopped off, each with 8 landmarks, given by the following configuration matrix

\[
\begin{pmatrix}
0 & 1 & \frac{1+\epsilon}{2} & \frac{1-\epsilon}{2} & 0 & 1 & \frac{1+\epsilon}{2} & \frac{1-\epsilon}{2} \\
0 & 0 & \frac{1+\epsilon}{2} & \frac{1-\epsilon}{2} & 1 & 1 & \frac{1+\epsilon}{2} & \frac{1-\epsilon}{2} \\
0 & 0 & \epsilon & \epsilon & 0 & 0 & \epsilon & \epsilon
\end{pmatrix}
\]

(cf. Figure 6) determined by \( \epsilon > 0 \). In the simulation, independent Gaussian noise is added to each landmark measurement. Table 3 gives the percentages of correct classifications.

![Figure 6: cube (left) and pyramid of varying height \( \epsilon \) (right) for classification.](image)

| \( \epsilon \) | intrinsic mean with tangent space coordinates |
|--------------|---------------------------------------------|
|              | intrinsic residual mean mean |
| 0.0          | 70\% 74\% 74\% 64\% |
| 0.2          | 56\% 58\% 57\% 51\% |
| 0.3          | 41\% 42\% 42\% 42\% |

Table 3: Percentage of correct classifications within 1,000 simulations each of 10 unit-cubes and 10 pyramids determined by \( \epsilon \) (which gives the height), where each landmark is independently corrupted by Gaussian noise of variance \( \sigma^2 = 0.2 \) via a Hotelling \( T^2 \)-test for equality of means to the significance level 0.05.

As visible from Table 3 discriminating flattened pyramids (\( \epsilon = 0 \)) from cubes (\( \epsilon = 1 \)) is achieved much better by employing intrinsic or Ziezold means
rather than Schoenberg means. This finding is in concord with Theorem 5.4: samples of size 10 of two-dimensional configurations yield Euclidean means a.s. in $\mathcal{P}^7$ which are projected to $\mathcal{P}^3$ to obtain Schoenberg means in $\Sigma^3_3$. In consequence, Schoenberg means of noisy nearly two-dimensional pyramids are essentially three dimensional. With increased height of the pyramid, ($\epsilon > 0$, i.e. for more pronounced third dimension and increased proximity to the unit cube) this effect waynes and all means perform equally well (or bad). Moreover in any case, intrinsic means with intrinsic tangent space coordinates qualify less for shape discrimination than intrinsic means with residual tangent space coordinates, cf. Remark 6.1. The latter (intrinsic means with residual tangent space coordinates) are better or equally well behaved as Ziezold means (which naturally use residual tangent space coordinates).

| intrinsic mean | Ziezold mean | Schoenberg mean |
|----------------|-------------|-----------------|
| 0.24           | 0.18        | 0.04            |

Table 4: Average time in seconds for the computation of means in $\Sigma^3_3$ of sample size 20 on a PC with a 800 MHZ CPU based on 1,000 repetitions.

In conclusion we record the time for the computations of means in Table 4. While Ziezold means compute in approximately $3/4$ of the computational time for intrinsic means, Schoenberg means are obtained approximately 6 times faster.

8 Discussion

By establishing stability results for intrinsic and Ziezold means on the manifold part of a shape space, a gap in asymptotic theory for general non-manifold shape spaces could be closed, now allowing for multi-sample tests of equality of intrinsic means and Ziezold means. A similar stability assertion in general is false for Procrustean means for low concentration. There is reason to believe, however, that it would be true for higher concentration. Note that the argument applied to intrinsic and Ziezold means fails for Procrustean means, since in contrast to the equations in Theorem 4.5 the sum of Procrustes residuals is in general non-zero. Loosely speaking, the findings on dimensionality condense to

- Procrustean means may decrease dimension by 2 or more,
- intrinsic and Ziezold means decrease dimension at most by 1, in particular, they preserve regularity,
- Schoenberg means tend to increase up to the maximal dimension possible.

Due to the proximity of Ziezold and intrinsic means on Kendall’s shape spaces in most practical applications, taking into account that the former are computationally easier accessable (optimally positioning and Euclidean averaging in every iteration step) than intrinsic means (optimally positioning and
weighted averaging in every iteration step), Ziezold means can be preferred over intrinsic means. They may be even more preferred over intrinsic means, since Ziezold means naturally come with residual tangent space coordinates which may allow in case of intrinsic means for a higher finite power of tests than intrinsic tangent space coordinates.

Computationally much faster (not relying on iteration at all) are Schoenberg means which are available for Kendall’s reflection shape spaces. As a drawback, however, Schoenberg means, seem less sensitive for dimensionality of configurations considered than intrinsic or Ziezold means. In particular for problems involving small sample sizes \( n \) and a large number of parameters \( p \) as currently of high interest in statistical applications, involving (nearly) degenerate data, Ziezold means may also be preferred over Schoenberg means due to higher power of tests.

Finally, note that Ziezold means may be defined for the shape spaces of planar curves introduced by Zahn and Roskies (1972), which are currently of interest e.g. Klassen et al. (2004) or Schmidt et al. (2006). Employing Ziezold means there, a computational advantage greater than found here can be expected since the computation of iterates of intrinsic means involves computations of geodesics which themselves can only be found iteratively.

Acknowledgment

The author would like to thank Alexander Lytchak for helpful advice on differential geometric issues.

A Proofs

**Lemma A.1.** Let \( U \subset M \) be a tubular neighborhood about \( p \in M \) that admits a slice via \( \exp_p D \times I_p G \cong U \) in optimal position to \( p \). Then, there is a measurable horizontal lift \( L \subset \exp_p D \) of \( \pi(U) \) in optimal position to \( p \).

**Proof.** If \( p \) is regular, then \( L = \exp_p D \) has the desired properties. Now assume that \( p \) is not of maximal orbit type. W.l.o.g. assume that \( D \) contains the closed ball \( B \) of radius \( r > 0 \) with bounding sphere \( S = \partial B \) and that there are \( p^1, \ldots, p^J \in \exp_p(S) \) having the distinct orbit types occurring in \( S \). \( S^j \) denotes all points on \( S \) of orbit type \( (G/I_p^j) \), \( j = 1, \ldots, J \), respectively. Observe that each \( S^j \) is a manifold on which \( I_p \) acts isometrically. Hence for every \( 1 \leq j \leq J \), there is a finite \( (K_j < \infty) \) or countable \( (K_j = \infty) \) sequence of tubular neighborhoods \( U^j_k \subset S^j \) covering \( S^j \), admitting trivial slices via

\[
\exp_{p^j_k}^{S^j} D^j_k \times I_p/I_{p^j_k} \cong U^j_k, \quad p^j_k \in U^j_k, \quad 1 \leq k \leq K_j.
\]

Here, \( \exp_{p^j_k}^{S^j} \) denotes the Riemannian exponential of \( S^j \). Defining a disjoint sequence

\[
\tilde{U}^j_1 := U^j_1, \quad \tilde{U}^j_{k+1} := U^j_{k+1} \setminus \tilde{U}^j_k \text{ for } 1 \leq k \leq K_j - 1
\]
exhausting $S^j$ we obtain a corresponding sequence of disjoint measurable sets $\exp_{p_k}^{S^j} \tilde{D}^j_k$ with
\[
\exp_{p_k}^{S^j} \tilde{D}^j_k \times I_p/I_{p_k} \cong \tilde{U}_k^j, \quad 1 \leq k \leq K_j.
\]
Hence, setting
\[
L^j_k := \exp_{p_k}^{S^j} \tilde{D}^j_k \quad \text{and} \quad L^j := \bigcup_{k=1}^{K_j} L^j_k
\]
observe that every $p' \in S^j$ has a unique lift in $L^j$ which is contained in a unique $L^j_k$. This lift is by construction (all $L^j_k$ are in $\exp_p(D)$ in optimal position to $p$). Moreover, if $p' \in L^j_k$ and $gp' \in L^j_k$ for some $g \in G$ with $1 \leq k', k \leq K_j$ we have by the disjoint construction of $\tilde{U}_k^j$ and $\tilde{U}_{k'}^j$ that $k = k'$, hence the isotropy groups of $gp'$ and $p'$ agree, yielding $gp' = p'$. In consequence, $L^j$ is a measurable horizontal lift of $S^j$ in optimal position to $p$. Since every horizontal geodesic segment $t \mapsto \exp_p(tv)$, $v \in H_pM$ contained in $\exp_p D$ features a constant isotropy group, except possibly for the initial point we obtain with the definition of
\[
L := \bigcup_{j=1}^J M^j \quad \text{with} \quad M^j := \{ \exp[(tu) \in \exp_p(D) : v \in \exp_p^{-1}(L^j), t \geq 0]\}
\]
a measurable horizontal lift of $\pi(U)$ in optimal position to $p$. \hfill \square

**Proof of Theorem 4.4.** Since $M$ is connected, any two points $p, p'$ can be brought into optimal position $p, gp'$ and a closed minimizing horizontal geodesic segment $\gamma_{gp'}$ between $p, gp'$ can be found. If $[p'] \in Q([p])$ then also $\gamma_{gp'} \subset Q([p])$. In consequence, there are tubulars neighborhoods $U_p$ of $p$ and $U_{p'}$ of $\gamma_{gp'}$, admitting slices in optimal position to $p$, which by Lemma A.1 have horizontal lifts $L_p$ and $L_{p'}$ in optimal position to $p$. Since $M$ is a manifold, there is a sequence $[p_0], \ldots \in Q([p])$, $g_j \in G, p_j \in M$ such that $p_0 = p$ and that each $g_jp_j$ is in optimal position to $p$ ($j \in J, J \subset \mathbb{N}$) and such that
\[
Q([p]) \subset \bigcup_{j \in J \cup \{0\}} \pi(U_{p_j})
\]
with measurable horizontal lifts $L_{p_j}$ of $\pi(U_{p_j})$. Defining $L^j_{p_0} := L_{p_0}$ and recursively $L^j_{p_{j+1}} := L^j_{p_{j+1}} \setminus L^j_{p_{j}}$ for $j = 1, \ldots$ a measurable horizontal lift $L' := \bigcup_{j=0}^\infty L^j_{p_0}$ of $Q([p])$ in optimal position to $p$ is obtained. Finally, suppose that $p_j$ is in optimal position to $p$ for $p_j \in [p_j] \in A$ and set $L'_0 := L'$, $L'_j := L'_{j-1} \cup \{p_j\}$ if $[p_j] \cap L'_j = \emptyset$ and $L'_j = L'_{j-1}$ ($j \geq 1$) otherwise to obtain the desired measurable horizontal lift $L'' := \bigcup_{[p_j] \in A} L''_j$ in optimal position to $p$.

**Proof of Theorem 4.7.** In case of intrinsic means, with the hypotheses and notations of the above proof of Theorem 4.4, suppose that $L''$ is a measurable horizontal lift of $Q([p]) \cup A$ in optimal position to an intrinsic mean $p \in M$ of the random element $Y$ on $M$ defined as in Theorem 4.5 with $[p] \in E(d_{ps})(X)$. For notational simplicity we assume that $Q([p]) = \pi(U)$ with a single tubular neighborhood $U$ of $p$ admitting a slice.
Then, additionally using the notation of the above proof of Lemma A.1, if the assertion of the Theorem would be false, w.l.o.g. there would be \( g \in I_p, 1 \leq j \leq J, p_j \in S^j \) with \( gp_j \neq p_j \) and \( \mathbb{P}\{Y \in M^j\} > 0 \). In particular, in the proof Lemma A.1 we may choose a sufficiently small \( U_j \) around \( p_j \) such that in consequence of (4)
\[
\int_{M_{k}^j(\epsilon)} \left( \exp_p^{-1} Y - \exp_p^{-1}(gY) \right) d\mathbb{P}_Y \neq 0 \tag{8}
\]
with some \( \epsilon > 0, M_{k}^j(\epsilon) := \{ \exp_p(tv) \in \exp_p(D) : v \in \exp_p^{-1}(L_{k}^j), |t - r| < \epsilon \} \) and \( L_{k}^j \) obtained from \( U_j \) as in the proof of Lemma A.1. Suppose that \( L \subset L'' \) is obtained as in the proof of Lemma A.1 by using \( L_{k}^j \) and suppose that \( L'' \) is obtained from \( L' \) by replacing the \( M_{k}^j(\epsilon) \) part of \( M_{k}^j \) with \( \{ \exp_p(tv) \in \exp_p(D) : v \in \exp_p^{-1}(gL_{k}^j), |t - r| < \epsilon \} \). Then \( L'' \) is also a measurable horizontal lift in optimal position to \( p \). Since we assume that \([p]\) is an intrinsic mean of \( X \), assertion (i) of Theorem 4.5 teaches that \( p \) is also an intrinsic mean of lift \( \tilde{Y} \) of \( X \) to \( L'' \), i.e.
\[
0 = \int_{L''} \exp_p^{-1} Y d\mathbb{P}_Y - \int_{L''} \exp_p^{-1} \tilde{Y} d\mathbb{P}_Y' = \int_{M_{k}^j(\epsilon)} \left( \exp_p^{-1} Y - \exp_p^{-1}(gY) \right) d\mathbb{P}_Y .
\]
This is a contradiction to (8) yielding the validity of the theorem for intrinsic means.

The assertion in case of Ziezold means is similarly obtained. Use the same horizontal lifts \( L'' \) and \( \tilde{L}'' \) from above, replace \( \exp_p^{-1} Y, \exp_p^{-1} \tilde{Y} \) and \( \exp_p^{-1}(gY) \) by \( df^{Y}_{ext}(p), df^{\tilde{Y}}_{ext}(p) \) and \( df^{gY}_{ext}(p) \), respectively, use the hypothesis (5) to obtain the analog of (8) and finally obtain the contradiction arguing with assertion (ii) of Theorem 4.5.

References

Afsari, B., 2010. Riemannian \( L^p \) center of mass: existence, uniqueness, and convexity. Proceedings of the American Mathematical Society 139, 655–773.

Bandulasiri, A., Patrangenaru, V., 2005. Algorithms for nonparametric inference on shape manifolds. Proc. of JSM 2005 Minneapolis, MN, 1617–1622.

Bhattacharya, A., 2008. Statistical analysis on manifolds: A nonparametric approach for inference on shape spaces. Sankhya, Ser. A 70 (2), 223–266.

Bhattacharya, R. N., Patrangenaru, V., 2003. Large sample theory of intrinsic and extrinsic sample means on manifolds I. Ann. Statist. 31 (1), 1–29.
Bhattacharya, R. N., Patrangenaru, V., 2005. Large sample theory of intrinsic and extrinsic sample means on manifolds II. Ann. Statist. 33 (3), 1225–1259.

Bredon, G. E., 1972. Introduction to Compact Transformation Groups. Vol. 46 of Pure and Applied Mathematics. Academic Press.

Choquet, G., 1954. Theory of capacities. Ann. Inst. Fourier 5, 131–295.

Dryden, I. L., Kume, A., Le, H., Wood, A. T. A., 2008. A multidimensional scaling approach to shape analysis. To appear.

Dryden, I. L., Mardia, K. V., 1998. Statistical Shape Analysis. Wiley, Chichester.

Fréchet, M., 1948. Les éléments aléatoires de nature quelconque dans un espace distancié. Ann. Inst. H. Poincaré 10 (4), 215–310.

Gower, J. C., 1975. Generalized Procrustes analysis. Psychometrika 40, 33–51.

Hendriks, H., Landsman, Z., 1996. Asymptotic behaviour of sample mean location for manifolds. Statistics & Probability Letters 26, 169–178.

Hendriks, H., Landsman, Z., 1998. Mean location and sample mean location on manifolds: asymptotics, tests, confidence regions. Journal of Multivariate Analysis 67, 227–243.

Hendriks, H., Landsman, Z., Ruymgaart, F., 1996. Asymptotic behaviour of sample mean direction for spheres. Journal of Multivariate Analysis 59, 141–152.

Huckemann, S., 2010a. Inference on 3D Procrustes means: Tree boles growth, rank-deficient diffusion tensors and perturbation models. Scand. J. Statist., to appear.

Huckemann, S., 2010b. R-package for intrinsic statistical analysis of shapes, http://www.mathematik.uni-kassel.de/~huckeman/software/ishapes_1.0.tar.gz.

Huckemann, S., Hotz, T., Munk, A., 2010a. Intrinsic MANOVA for Riemannian manifolds with an application to Kendall’s space of planar shapes. IEEE Transactions on Pattern Analysis and Machine Intelligence 32 (4), 593–603.

Huckemann, S., Hotz, T., Munk, A., 2010b. Intrinsic shape analysis: Geodesic principal component analysis for Riemannian manifolds modulo Lie group actions (with discussion). Statistica Sinica 20 (1), 1–100.

Huckemann, S., Ziezold, H., 2006. Principal component analysis for Riemannian manifolds with an application to triangular shape spaces. Adv. Appl. Prob. (SGSA) 38 (2), 299–319.

Jupp, P. E., 1988. Residuals for directional data. J. Appl. Statist. 15 (2), 137–147.
Karcher, H., 1977. Riemannian center of mass and mollifier smoothing. Communications on Pure and Applied Mathematics XXX, 509–541.

Kendall, D., 1974. Foundations of a theory of random sets. Stochastic Geom., Tribute Memory Rollo Davidson, 322-376 (1974).

Kendall, D. G., Barden, D., Carne, T. K., Le, H., 1999. Shape and Shape Theory. Wiley, Chichester.

Kendall, W. S., 1990. Probability, convexity, and harmonic maps with small image I: Uniqueness and fine existence. Proc. London Math. Soc. 61, 371–406.

Klassen, E., Srivastava, A., Mio, W., Joshi, S., Mar. 2004. Analysis on planar shapes using geodesic paths on shape spaces. IEEE Transactions on Pattern Analysis and Machine Intelligence 26 (3), 372–383.

Kobayashi, S., Nomizu, K., 1963. Foundations of Differential Geometry. Vol. I. Wiley, Chichester.

Kobayashi, S., Nomizu, K., 1969. Foundations of Differential Geometry. Vol. II. Wiley, Chichester.

Krim, H., Yezzi, A. J. J. E., 2006. Statistics and Analysis of Shapes. Modeling and Simulation in Science, Engineering and Technology. Birkhäuser, Boston.

Le, H., 2001. Locating Fréchet means with an application to shape spaces. Adv. Appl. Prob. (SGSA) 33 (2), 324–338.

Le, H., 2004. Estimation of Riemannian barycenters. LMS Journal of Computation and Mathematics 7, 193–200.

Mardia, K., Patrangenaru, V., 2001. On affine and projective shape data analysis. Functional and Spatial Data Analysis, Proceedings of the 20th LASR Workshop (Eds: K.V. Mardia and R.G. Aykroyd), 39–45.

Mardia, K., Patrangenaru, V., 2005. Directions and projective shapes. Ann. Statist. 33, 1666–1699.

Matheron, G., 1975. Random sets and integral geometry. Wiley Series in Probability and Mathematical Statistics. New York.

Nash, J., 1956. The imbedding problem for Riemannian manifolds. Ann. of Math. 63, 20–63.

Palais, R. S., 1961. On the existence of slices for actions of non-compact Lie groups. Ann. Math. 2nd Ser. 73 (2), 295–323.

Schmidt, F. R., Clausen, M., Cremers, D., 2006. Shape matching by variational computation of geodesics on a manifold. In: Pattern Recognition (Proc. DAGM). Vol. 4174 of LNCS. Springer, Berlin, Germany, pp. 142–151.
Small, C. G., 1996. The Statistical Theory of Shape. Springer-Verlag, New York.

Zahn, C., Roskies, R., 1972. Fourier descriptors for plane closed curves. IEEE Trans. Computers C-21, 269–281.

Ziezold, H., 1977. Expected figures and a strong law of large numbers for random elements in quasi-metric spaces. Trans. 7th Prague Conf. Inf. Theory, Stat. Dec. Func., Random Processes A, 591–602.

Ziezold, H., 1994. Mean figures and mean shapes applied to biological figure and shape distributions in the plane. Biom. J. (36), 491–510.
On the Meaning of Mean Shape

Stephan Huckemann

Abstract

A stability result for intrinsic means on the quotient due to an isometric and proper Lie group action on a Riemannian manifold is derived, stating that intrinsic means are contained in the highest dimensional manifold stratum assumed with non-zero probability. In consequence, the Central Limit Theorem (CLT) for manifold valued random elements can be extended to non-manifold shape spaces. The relationship to other types of means is discussed: the CLT extends to Ziezold means but not in general to Procrustes means, since the latter may be contained in lower dimensional manifold strata. In contrast, Schoenberg means tend to increase dimension. The finite power of tests may increase when switching from intrinsic tangent space coordinates to residual tangent space coordinates. This and computational speed makes Ziezold means most competitive for multi-sample test. Curiously, intrinsic, Ziezold, and Procrustes means are related in such that in approximation the Ziezold means divides the generalized geodesic segment between intrinsic and Procrustes mean by the ratio $1:3$. Classical data-sets as well as numerical simulations illustrate the findings.

Key words and phrases: Shape Spaces, Intrinsic Mean, Extrinsic Mean, Mean Location, Stability, General Procrustes Analysis, Full Procrustes Mean, Isometric Group Action, Schoenberg Mean, Power of Tests

Figure AMS 2000 Subject Classification: Primary 60D05
Secondary 62H11

1 Introduction

The analysis of shape may be counted among the very early activities of mankind; be it for representation on cultural artefacts, or for morphological, biological and medical application, to name only two of its driving forces. In modern days shape analysis is gaining increased momentum in computer vision, image analysis, biomedicine and many other fields. For a fairly recent overview over key aspects cf. [Krim and Yezzi (2006)]. To begin with, already the concept of an expected, averaged or mean shape is surprisingly non trivial and not at all canonical. This is due to the fact that spaces of shapes usually admit several natural structures, and, in many cases none of them is that of a Euclidean space. While some structures are Euclidean (e.g. [Mosimann (1970)],...
structures that may be considered benign are that of Riemannian manifolds (e.g. Blum and Nagel (1978), Kendall (1984)). Many shape spaces, however, admit only the structure of a Riemannian manifold – the \textit{pre-shape space} of configurations – modulo the isometric action of a Lie group, conveying shape equivalence. We call the quotient a \textit{shape space}. It carries a canonical quotient structure of a union of manifold strata of different dimensions, which give in general a Riemannian manifold – the \textit{manifold part} – with singularities at some of which the curvature may tend to infinity. Prominent examples are Kendall’s three- and higher-dimensional shape spaces, cf. Kendall et al. (1999), and the spaces of closed planar curves, see Zahn and Roskies (1972).

In a Euclidean space, there is a clear and unique concept of a mean in terms of least squares minimization: the arithmetic average. Generalizing to manifolds, however, with every embedding in a Euclidean space come specific concepts of extrinsic means and residual means, and with every manifold structure a specific concept of an intrinsic mean. Carrying statistics over to manifolds, strong consistency and central limit theorems (CLTs) for extrinsic, residual and intrinsic means have been derived by Jupp (1988), Hendriks and Landsman (1994, 1998) as well as by Bhattacharya and Patrangenaru (2003, 2005). Under quotienting these means generalize to Ziezold means and Procrustes means, respectively, and again, to intrinsic means. For a CLT to hold, obviously, a manifold structure is inevitable. Due to strong consistency, which has been established by Ziezold (1977) on general quasi-metrical spaces, for a \textit{one-sample test} for a specific mean shape on the manifold part, it may be assumed that sample means eventually lie on the manifold part as well, thus making the above CLT available. Multi-sample tests, however, could not be theoretically justified because it remained unclear whether means of random shapes on the manifold part come to lie on the manifold part again.

As the key result in this paper it is shown that intrinsic and Ziezold means lie on the manifold part whenever the manifold part is assumed with non-zero probability. In consequence the CLT for manifolds can be applied in general, thus making multi-sample tests for these mean shapes possible. We note that specifically for the non-manifold Kendall reflection shape spaces, Schoenberg means as have been recently introduced by Bandulasiri and Patrangenaru (2005) as well as by Dryden et al. (2008) also allow for asymptotic inference.

This paper is structured as follows. In motivation in Section 2 Kendall’s shape spaces are introduced along with the specific application of the key result. The following Section 3 lays out the various concepts of means in a generic shape space setting. In Section 4 the stability theorem, namely that

\textit{intrinsic means preserve dimension}

is established. The proof is based on lifting a distribution on the shape space to the pre-shape space and subsequently exploiting the fact that intrinsic means are zeroes of an integral involving the Riemann exponential. The similar argument can be applied to Ziezold means but not to Procrustes means. The population case is more intrigued, however, as the lifting requires the concept of tubular
neighborhoods admitting slices. In Section 5 extrinsic means are discussed, in particular that Schoenberg means are due to a non-isometric embedding and that they tend to “increase the dimension”. Section 6 tackles local effects of curvature: Section 6.1 motivates why residual tangent space coordinates may yield a higher finite power than intrinsic tangent space coordinates. The closeup on spherical means in Section 6.2 reveals that, if the following means are unique, the generalized geodesic segment between the intrinsic mean and the Procrustes mean (closer to the data) is in approximation divided by the Ziezold mean by the ration $1 : 3$. Section 7 illustrates the practical effects of the theoretical results using classical data-sets as well as simulations.

2 Motivation: Kendall’s Shape Spaces

In the statistical analysis of similarity shapes based on landmark configurations, geometrical $m$-dimensional objects (usually $m = 2,3$) are studied by placing $k > m$ landmarks at specific locations of each object. Each object is then described by a matrix in the space $M(m,k)$ of $m \times k$ matrices, each of the $k$ columns denoting an $m$-dimensional landmark vector. $(x,y) := \text{tr}(xy^T)$ denotes the usual inner product with norm $\|x\| = \sqrt{\langle x,x \rangle}$. For convenience and without loss of generality for the considerations below, only centered configurations are considered. Centering can be achieved by multiplying with a sub-Helmetr matrix $H \in M(k,k-1)$ from the right, yielding a configuration $xH$ in $M(m,k-1)$.

For this and other centering methods cf. Dryden and Mardia (1998, Chapter 2). Excluding also all configurations with all landmarks coinciding gives the space of configurations

$$F^k_m := M(m,k-1) \setminus \{0\}.$$ 

Since only the similarity shape is of concern, we may assume that all configurations are contained in the unit sphere $S^k_m := \{x \in M(m,k-1) : \|x\| = 1\}$. Then, Kendall’s shape space is the canonical quotient

$$\Sigma^k_m := S^k_m / SO(m) = \{[x] : x \in S^k_m\}$$

with the fiber $[x] = \{gx : g \in SO(m)\}$.

In some applications reflections are also filtered out giving Kendall’s reflection shape space

$$R\Sigma^k_m := \Sigma^k_m / \{e, \tilde{e}\} = S^k_m / O(m).$$

Here, $O(m) = \{g \in M(m,m) : g^Tg = e\}$ denotes the orthogonal group with the unit matrix $e = \text{diag}(1,\ldots,1)$, $\tilde{e} = \text{diag}(-1,1,\ldots,1)$ and $SO(m) = \{g \in O(m) : \det(g) = 1\}$ is the special orthogonal group.

For $1 \leq j \leq m < k$ consider the (non-unique) embedding

$$S^k_j \hookrightarrow S^k_m : x \mapsto \begin{pmatrix} x \\ 0 \end{pmatrix} \quad (1)$$

giving rise to a unique and canonical embedding of $\Sigma^k_j \hookrightarrow \Sigma^k_m$, which is isometric w.r.t. the canonical intrinsic distance, the Procrustes distance and the Ziezold
distance defined in Section 3, cf. Kendall et al. (1999, pp. 29, 206). In consequence, intrinsic means, Procrustes means and Ziezold means (also defined in Section 3) of random elements taking values in $\Sigma^k_j \subset \Sigma^k_m$, are also contained within $\Sigma^k_j$:

Remark 2.1. Suppose that $[X]$ is a random shape on $\Sigma^k_m$ assuming shapes of configurations of dimension less than or equal to $j$ ($1 \leq j \leq m$) with probability one, then every intrinsic, Procrustes and Ziezold mean shape of $[X]$ corresponds to a configuration of dimension less than or equal to $j$.

The main result of this paper in form Corollaries 4.4 and 4.9 applied to Kendall’s spaces states that intrinsic and Ziezold means are also non-decreasing in dimension. In view of Ziezold means, Remark 3.4 provides invariant optimal positioning and (3) on page 8 is valid on the pre-shape sphere. The technical definition of a cut locus on the quotient and a tubular neighborhood admitting a slice can be found in Section 4.1.

Theorem 2.2 (Intrinsic and Ziezold Kendall Means Preserve Dimension). Suppose that $[X]$ is a random pre-shape on $\Sigma^k_m$, $m > k$ with intrinsic or Ziezold mean shape $[\mu] \in \Sigma^k_m$, $\mu \in S^k_m$. Moreover suppose that $[X]$ either assumes discrete values outside the cut locus of $[\mu]$ a.s. or that it is supported by a projection of a tubular neighborhood around $\mu$ admitting a slice. If $[X]$ assumes shapes corresponding to non-degenerate configurations up to dimension $j$ ($1 \leq j \leq m$) with non-zero probability then $\mu$ corresponds to a non-degenerate $j$-dimensional configuration.

3 Fréchet $\rho$-means and General Shape Spaces

In the previous section we introduced Kendall’s shape and reflection shape space based on invariance under similarity transformations; e.g. invariance under congruence transformations only leads to Kendall’s size-and-shape space. More generally, in image analysis, invariance may also be considered under the affine or projective group, cf. Mardia and Patrangenaru (2001, 2005); Munk et al. (2008). A different yet also very popular popular set of shape spaces for two-dimensional configurations modulo the group of similarities has been introduced by Zahn and Roskies (1972). Instead of building on a finite dimensional Euclidean matrix space modeling landmarks, the basic ingredient of these spaces modeling closed planar unit speed curves is the infinite dimensional Hilbert space of Fourier series. In practice for numerical computation, only finitely many Fourier coefficients are considered.

To start with, a shape space is a metric space $(\mathbb{Q}, d)$. For this entire paper suppose that $X, X_1, X_2, \ldots$ are i.i.d. random elements mapping from an abstract probability space $(\Omega, \mathcal{A}, \mathbb{P})$ to $(\mathbb{Q}, d)$ equipped with its self understood Borel $\sigma$-field. Moreover, denote by $\mathbb{E}(Y)$ the classical expected value of a random element $Y$ on a $D$-dimensional Euclidean space $\mathbb{R}^D$, if existent.
Definition 3.1. For a continuous function $\rho : Q \times Q \to [0, \infty)$, define the set of population Fréchet $\rho$-means by

$$E^{(\rho)}(X) = \arg\min_{\mu \in Q} \mathbb{E}(\rho(X, \mu)^2).$$

For $\omega \in \Omega$ denote by

$$E^{(\rho)}_n(\omega) = \arg\min_{\mu \in Q} \sum_{j=1}^n \rho(X_j(\omega), \mu)^2$$

the set of sample Fréchet $\rho$-means.

By continuity of $\rho$, the mean sets are closed random sets. For our purpose here, we rely on the definition of random closed sets as introduced and studied by Choquet [1954], Kendall [1974] and Matheron [1975]. Since their original definition for $\rho = d$ by Fréchet [1948] such means have found much interest.

Intrinsic means. Independently, for a Riemannian manifold with geodesic distance $d = \rho$, Kobayashi and Nomizu [1969] defined the corresponding means as centers of gravity which are nowadays also well known as intrinsic means (Bhattacharya and Patrangenaru [2003, 2005]).

Extrinsic means. W.r.t. the chordal or extrinsic metric $d = \rho$ due to an embedding of a Riemannian manifold in an ambient Euclidean space, such means have been called mean locations by Hendriks [1991] or extrinsic means by Bhattacharya and Patrangenaru [2003].

More precisely, let $Q = M \subset \mathbb{R}^D$ be a Riemannian manifold embedded in a Euclidean space $\mathbb{R}^D$ and let $\Phi : \mathbb{R}^D \to M$ denote the orthogonal projection, $\Phi(x) = \inf_{\mu \in M} \|x - \mu\|$. For any Riemannian manifold an embedding that is even isometric can be found for $D$ sufficiently large, see Nash [1956]. Due to an extension of Sard’s Theorem by Bhattacharya and Patrangenaru [2003, p.12] for a closed manifold, $\Phi$ is uni-valent up to a set of Lebesgue measure zero. Then the set of extrinsic means is given by the set of images $\Phi(E(Y))$ where $Y$ denotes $X$ viewed as taking values in $\mathbb{R}^D$ (cf. Bhattacharya and Patrangenaru [2003]).

Residual means. In this context, setting $\rho(p, q) = \|d\Phi_q(p - q)\|$ $(p, q \in M)$ with the derivative $d\Phi_q$ at $q$ yielding the orthogonal projection to the embedded tangent space $T_q\mathbb{R}^D \to T_qM \subset T_q\mathbb{R}^D$, call the corresponding mean sets $E^{(\rho)}(X)$ and $E^{(\rho)}_n(\omega)$, the sets of residual population means and residual sample means, respectively. For two-spheres, $\rho(p, q)$ has been studied under the name of crude residuals by Jupp [1988]. In general, on unit-spheres

$$\rho(p, q) = \|p - \langle p, q \rangle q\| = \sqrt{1 - \langle p, q \rangle^2} = \rho(q, p)$$

is a quasi-metric (symmetric, vanishing on the diagonal $p = q$ and satisfying the triangle inequality).
Due to curvature these concepts of means are essentially non-convex in the following sense.

**Remark 3.2.** To a random point on a two-sphere, uniformly distributed along its equator, both north and south pole are intrinsic and extrinsic means.

Residual means, however, seem less affected.

**Theorem 3.3.** If a random point $X$ on a unit sphere is a.s. contained in a unit subsphere $S$ then $S$ contains as well every residual mean of $X$.

**Proof.** Suppose that $x = v + \nu$ is a residual mean of $X$ with $v/\|v\| \in S$ and $\nu$ normal to $S$. Since $1 - (X, v + \nu)^2 = 1 - (X, v)^2 \geq 1 - (X, v)^2/\|v\|^2$ a.s. with equality if and only if $\nu = 0$, the assertion follows at once from (2).

Let us now incorporate more of the structure common to shape spaces: $M$ is a complete connected $D$-dimensional Riemannian manifold with geodesic distance $d_M$ on which a Lie group $G$ acts properly and isometrically from the left. Then we call the canonical quotient

$$\pi : M \to Q := M/G = \{ [p] : p \in M \}$$

where $[p] = \{ gp : g \in G \}$, a shape space. As a consequence of the isometric action we have that $d_M(gp, q) = d(p, g^{-1}q)$ for all $p, q \in M, g \in G$. For $p, q \in M$ we say that $p$ is in optimal position to $q$ if $d_M(p, q) = \min_{g \in G} d_M(gp, q)$, the minimum is attained in consequence of the proper action. As is well known (e.g. Bredon (1972, p. 179)) there is an open and dense submanifold $M^*$ of $M$ such that the canonical quotient $Q^* = M^*/G$ restricted to $M^*$ carries a natural manifold structure also being open and dense in $Q$. Elements in $M^*$ and $Q^*$, respectively, are called regular, the complementary elements are singular; $Q^*$ is the manifold part.

**Intrinsic means on shape spaces.** The canonical distance

$$d_Q([p], [q]) := \min_{g \in G} d_M(gp, q) = \min_{g, h \in G} d_M(gp, hq)$$

is called intrinsic distance and the corresponding $d_Q$-Fréchet mean sets are called intrinsic means. Note that the intrinsic distance is equal to the canonical geodesic distance on $Q^*$.

**Ziezold and Procrustes means.** Now, assume that we have an embedding with orthogonal projection $\Phi : \mathbb{R}^D \to M \subset \mathbb{R}^D$ as above. If the action of $G$ is isometric w.r.t. the extrinsic metric, i.e. if $\| gp - gq \| = \| p - q \|$ for all $p, q \in M$ and $g \in G$ then call

$$\rho_Q^{(z)}([p], [q]) := \min_{g \in G} \| gp - q \|$$

$$\rho_Q^{(p)}([p], [q]) := \min_{g \in G} \| d\Phi g(gp - q) \|$$
the Ziezold distance and the Procrustes distance on $Q$, respectively. The corresponding Fréchet mean sets are the Ziezold means and the Procrustes means, respectively. We say that optimal positioning is invariant if

$$d_M(g^*p, q) = \min_{g \in G} d_M(gp, q) \Leftrightarrow \|g^*p - q\| = \min_{g \in G} \|gp - q\|$$

for all $p, q \in M$ and $g^* \in G$.

Remark 3.4. Indeed for $Q = \Sigma_m^k$, optimal positioning is invariant (cf. Kendall et al. (1999, p. 206)). Procrustes means coincide with classical Procrustes means introduced by Gower (1975) and Ziezold means coincide with means as introduced by Ziezold (1994). Moreover for $Q = \Sigma_2^k$, Procrustes means agree with extrinsic means w.r.t. the Veronese-Whitney embedding, cf. Bhattacharya and Patrangenaru (2003) and Section 5.

4 Stability Results for Intrinsic Means

In this section we derive the stability results underlying Theorem 2.2. To this end we need to recall how a non-manifold shape space is made up from manifold strata of varying dimensions.

4.1 Preliminaries

As before, let $M$ be a complete connected Riemannian manifold called the pre-shape space with intrinsic metric $d_M$ on which a Lie group $G$ acts properly and isometrically giving rise to the canonical quotient $Q = M/G$ called the shape space with intrinsic metric $d_Q$. The canonical projection is denoted by $\pi : M \to Q$. $T_pM$ is the tangent space of $M$ at $p \in M$ and $\exp_p$ denotes the Riemannian exponential at $p$. On a complete and connected manifold $M$ we have for every $p' \in M$ that there is $v' \in T_pM$ such that $p' = \exp_p v'$. $v' = \exp_{p'}^{-1} p'$ of minimal modulus is uniquely determined as long as $p \in M \setminus C(p)$ with the cut locus $C(p)$ of $p$ which is a subset of measure zero in $M$. E.g. on a sphere, the cut locus of any point is its antipode. For $q \in Q$ let

$$C(q) := \{p' : p' \in C(p) \text{ is in optimal position to some } p \in q\}$$

be the cut locus on the quotient of $q \in Q$.

Next we recollect consequences of the Lie group action, see Bredon (1972). The stability result in the sample case (below in Section 4.2) rests on (A) and (B) alone.

(A) With the isotropy group $I_p = \{g \in G : gp = p\}$ for $p \in M$, every orbit carries the natural structure of a coset space $[p] \cong G/I_p$. Moreover, $p' \in M$ is of orbit type $(G/I_p)$ if $I_{p'} = gI_pg^{-1} = I_{gp}$ for a suitable $g \in G$. If $I_p \subset I_{gp'}$ for suitable $g \in G$ then $p'$ is of lower orbit type than $p$. 

7
(B) The pre-shapes of equal orbit type

\[ M^{(I_p)} := \{ p' \in M : p' \text{ is of orbit type } (G/I_p) \} \]

and the corresponding shapes \( Q^{(I_p)} := \{ [p'] : p' \in M^{(I_p)} \} \) are manifolds in \( M \) and \( Q \), respectively.

(C) The orthogonal complement \( H_pM \) in \( T_pM \) of the tangent space \( T_p[p] \) along the orbit is called the horizontal space: \( T_pM = T_p[p] \oplus H_pM \).

(D) The Slice Theorem (cf. Palais (1960)) states that every \( p \in M \) has a tubular neighborhood \( [p] \subset U \subset M \) such that with a suitable open subset \( D \subset H_pM \) the twisted product \( \exp_p D \times [p] \) is diffeomorphic with \( U \). Here, the twisted product is the natural topological quotient of the product space \( \exp_p D \times [p] \) modulo the equivalence

\[ (\exp_p v, gp) \sim_{I_p} (\exp_p v', g'p) \iff \exists h \in I_p \text{ such that } v' = dhv, \ g' = gh^{-1}. \]

For short we say that the tubular neighborhood \( U \) admits a slice \( \exp_p D \) through \( p \).

(E) If a tubular neighborhood \( U \) of \( p \) admits a slice \( \exp_p D \) then every \( p' \in \exp_p D \) is in optimal position to \( p \). Moreover, all points \( p' \in U \) are of orbit type larger than or equal to the orbit type of \( p \) and only finitely many orbit types occur in \( U \). If \( p \) is regular, i.e. of maximal orbit type, then the quotient is trivial: \( \exp_p D \times [p] = \exp_p D \times [p] \).

Finally, we link intrinsic to Ziezold means. The gradient of the mapping \( f_{int} : T_pM \to [0, \infty) \) defined by \( f_{int}^{(p)}(v) = d_M(p, \exp_p v)^2 \) is given by \( \text{grad } f_{int}^{(p)}(v) = 2v \).

Hence, we have for \( p_1, p_2 \in M \setminus C(p) \) that

\[ \text{grad } f_{int}^{(p)}(\exp_p^{-1} p_1) = \text{grad } (f_{int}^{(p)})(\exp_p^{-1} p_2) \iff p_1 = p_2 \]

In view of Ziezold means let \( f_{ext}^{(p)} : T_pM \to [0, \infty) \) be defined by \( f_{ext}^{(p)}(v) = \|p - \exp_p v\|^2/2 \). Mimicking the above property introduce the following condition

\[ \text{grad } (f_{ext}^{(p)})(\exp_p^{-1} p_1) = \text{grad } (f_{ext}^{(p)})(\exp_p^{-1} p_2) \iff p_1 = p_2 \quad (3) \]

for \( p_1, p_2 \in M \setminus C(p) \). E.g. on spheres, \( \text{grad } \) is only true on half-spheres.

### 4.2 Stability of Sample Means

For short, for sampled points \( p_1, \ldots, p_n \in M \) denote the set of intrinsic or extrinsic sample means, respectively, by \( E(p_1, \ldots, p_n) \); similarly for \( q_1, \ldots, q_n \in Q \) denote the set of intrinsic or Ziezold sample means, respectively, by \( E(q_1, \ldots, q_n) \). Obviously, both sets are non-void.
Lemma 4.1. In case of extrinsic and Ziezold means assume that optimal positioning is invariant. Let \( q_1, \ldots, q_n \in Q \) and \( p_1, \ldots, p_n \in q_n \) are in optimal position to \( \overline{q} \) then \( \overline{p} \in E(p_1, \ldots, p_n) \).

Proof. The proof in case of extrinsic and Ziezold means is completely analogous to the following case of intrinsic means. If the assertion would not be true, we would have with \( p \in E(p_1, \ldots, p_n) \) that

\[
\sum_{j=1}^{n} d_Q([p], q_j)^2 = \sum_{j=1}^{n} d_M(p, g_j p_j)^2 < \sum_{j=1}^{n} d_M(\overline{q}, p_j)^2 = \sum_{j=1}^{n} d_Q(q, q_j)^2
\]

for \( g_1 p_1, \ldots, g_n p_n \) in optimal position to \( p \), a contradiction to the hypothesis \( \overline{q} \in E(q_1, \ldots, q_n) \). \( \square \)

The following necessary condition is taken from (Kobayashi and Nomizu, 1969, p. 110).

Lemma 4.2. In case of intrinsic means let \( \overline{p} \in M \) and \( p_1, \ldots, p_n \in M \setminus C(\overline{p}) \) with \( \overline{p} \in E(p_1, \ldots, p_n) \) for a complete and connected manifold \( M \). Then

\[
\sum_{j=1}^{n} \exp_{\overline{p}}^{-1} p_j = 0.
\]

For extrinsic means the analog condition is

\[
\sum_{j=1}^{n} f_{\overline{p}}^{\overline{p}}(\overline{p}, \exp_{\overline{p}}^{-1} p_j) = 0. \tag{4}
\]

Theorem 4.3. Suppose that \( G \) is a Lie group acting properly and isometrically on a complete connected Riemannian manifold \( M \) giving rise to the natural quotient \( Q = M/G \). If \( \overline{q} \in E(q_1, \ldots, q_n) \) is an intrinsic sample mean of \( q_1, \ldots, q_n \in Q \setminus C(\overline{q}) \) then

\[
I_{\overline{p}} \subset \cap_{j=1}^{n} I_{p_j},
\]

with arbitrary \( \overline{p} \in \overline{q} \) and \( p_1, \ldots, p_n \in q_n \) in optimal position to \( \overline{p} \). In case of invariant optimal positioning and under condition (3) the same assertion is true if \( \overline{q} \) is a Ziezold sample mean.

Proof. The proof in case of Ziezold means is completely analogous to the following case of intrinsic means, using (1) instead of Lemma 4.2. If the assertion would be false, we may assume that \( I_{\overline{p}} \not\subset I_{p_1} \), i.e. that there is \( g \in G \) with \( g \overline{p} = \overline{p} \) but \( g p_1 \neq p_1 \). In consequence of Lemma 4.1 \( \overline{p} \) is an intrinsic mean of both \( p_1, \ldots, p_n \) and \( gp_1, gp_2, \ldots, p_n \), both being in optimal position to \( \overline{p} \). Since
by hypothesis, \( \exp_{g_1}^{-1}(g p_1) \neq \exp_{p_1}^{-1}(p_1) \) is well defined, we have in consequence of Lemma 4.2 the contradiction
\[
0 = \exp_{g_1}^{-1}g p_1 + \sum_{j=2}^{n} \exp_{p_j}
= \exp_{g_1}^{-1}g p_1 - \exp_{p_1}^{-1}p_1 + \sum_{j=1}^{n} \exp_{p_j} \neq 0.
\]

\[\square\]

**Corollary 4.4.** Suppose that \( G \) is a Lie group acting properly and isometrically on a complete connected Riemannian manifold \( M \) giving rise to the natural quotient \( Q = M/G \). Then every intrinsic mean \( \bar{q} \in Q \) of a sample \( q_1, \ldots, q_n \in Q \setminus C(q) \) is regular if the sample contains at least one regular point. In case of invariant optimal positioning and under condition (3) the same assertion is true for Ziezold sample means.

**Proof.** The assertion is a consequence of Theorem 4.3 and the well known fact that regular points \( p^* \in M^* \) are characterized by the property that for every \( p \in M \) there is a \( g = g_p \in G \) such that \( g I_p g^{-1} \subseteq I_p \); if additionally \( p \) is in optimal position to \( p^* \) then \( g \in I_p \). \[\square\]

### 4.3 Stability of Population Means

**Theorem 4.5.** Assume that \( X \) is a random element on the canonical quotient \( Q = M/G \) due to the isometric and proper action of a Lie group \( G \) on a complete Riemannian manifold \( M \). Let \( p \in M \) and suppose that \( X \) is supported on \( \pi(U) \) with a tubular neighborhood \( U \subseteq M \) of \( [p] \) that admits a slice \( \exp_p \mathbb{R} \times I_p \) \( [p] \cong U \), \( D \in H_p M \). If \( P\{X \in Q(I_{p'})\} \neq 0 \) for some \( p' \in U \) and if either \([p]\)

(i) is an intrinsic mean of \( X \) or

(ii) is a Ziezold mean of \( X \) while optimal positioning is invariant and (3) is valid,

then \( p' \) is of lower orbit type than \( p \).

The proof of Theorem 4.5 further below relies on the two following lemmas for which we first develop an additional concept.

In the following, **measurable** will refer to the corresponding Borel \( \sigma \)-algebras, respectively.

**Definition 4.6.** Call a measurable subset \( L \subset M \) a **measurable horizontal lift** of a subset \( R \) of \( M/G \) in optimal position to \( p \in M \) if

1. the canonical projection \( L \to R \subset M/G \) surjective,

2. every \( p' \in L \) is in optimal position to \( p \),
3. every orbit \([p']\) of \(p' \in L\) meets \(L\) once.

**Lemma 4.7.** Let \(U \subset M\) be a tubular neighborhood about \(p \in M\) that admits a slice \(\exp_p D \times I_p[p] \cong U\). Then, there is a measurable horizontal lift \(L \subset \exp_p D\) of \(\pi(U)\).

**Proof.** If \(p\) is regular, then \(L = \exp_p D\) has the desired properties, cf. (E) above. Now assume that \(p\) is not of maximal orbit type. W.l.o.g. assume that \(D\) contains the closed ball \(B\) of radius \(r > 0\) with bounding sphere \(S = \partial B\) and that there are \(p_1, \ldots, p_J \in \exp_p(S)\) having the distinct orbit types occuring in \(S\). \(S^j\) denotes all points on \(S\) of orbit type \((G/I_p), j = 1, \ldots, J\), respectively. Observe that each \(S^j\) is a manifold on which \(I_p\) acts properly and isometrically. Hence for every \(1 \leq j \leq J\), there is a finite \((K_j < \infty)\) or countable \((K_j = \infty)\) sequence of tubular neighborhoods \(U^j_k \subset S^j\) covering \(S^j\), admitting trivial slices

\[
\exp^{S^j}_{p_k} D^j_k \times \{gp^j_k : g \in I_{p_k}\} \cong U^j_k, \quad 1 \leq k \leq K_j.
\]

Here, \(\exp^{S^j}_{p_k}\) denotes the Riemann exponential of \(S^j\). Defining a disjoint sequence

\[
\tilde{U}^j_1 := U^j_1 \\
\tilde{U}^j_{k+1} := U^j_{k+1} \setminus \tilde{U}^j_k \quad \text{for} \quad 1 \leq k \leq K_j - 1
\]

exhausting \(S^j\) we obtain a corresponding sequence of disjoint measurable sets \(\tilde{D}^j_k\) with

\[
\exp^{S^j}_{p_k} \tilde{D}^j_k \times \{gp^j_k : g \in I_{p_k}\} \cong \tilde{U}^j_k, \quad 1 \leq k \leq K_j.
\]

Setting

\[
L^j_k := \exp^{S^j}_{p_k} \tilde{D}^j_k \quad \text{and} \quad L^j := \bigcup_{k=1}^{K_j} L^j_k
\]

observe that every \(p' \in S^j\) has a unique lift in \(L^j\) which is contained in a unique \(L^j_k\). This lift is by construction in optimal position to \(p\). If \(gp' \in L^j_{k'}\) for some \(g \in G\) and \(1 \leq k' \leq K_j\) we have by the disjoint construction of \(\tilde{U}^j_k\) and \(\tilde{U}^j_{k'}\) that \(k = k'\), hence the isotropy groups of \(gp'\) and \(p'\) agree, yielding \(gp' = p'\). In consequence, \(L^j\) is a measurable horizontal lift of \(S^j\) in optimal position to \(p\).

Since every horizontal geodesic segment \(t \mapsto \exp_p(tv), v \in H_p M\) contained in \(\exp_p D\) features a constant isotropy group, except possibly for the initial point we obtain with the definition of

\[
L := \{\exp_p(tv) \in \exp_p D : v \in \exp_{p}^{-1}(L^j)\} \quad \text{for some} \quad 1 \leq j \leq J, t \geq 0
\]

a measurable horizontal lift of \(\pi(U)\) in optimal position to \(p\).

The following Lemma 4.8 is the analog in the population case of Lemmas 4.1 and 4.2. The proof goes similar.
Lemma 4.8. Assume that $X$ is a random element on the canonical quotient $Q = M/G$ due to the isometric and proper action of a Lie group $G$ on a complete Riemannian manifold $M$. Moreover, assume that there is $p \in M$ with tubular neighborhood $U \subset M$ of $[p]$ that admits a slice $\exp_p D \times t_p [p] \cong U$ such that $X$ is supported by $\pi(U)$. With a measurable horizontal lift $L$ of $\pi(U)$ define the random element $Y$ on $L \subset M$ by $\pi \circ Y = X$. If $[p]$ is an intrinsic mean of $X$ on $Q$, then $p$ is an intrinsic mean of $Y$ on $M$ and
\[ \mathbb{E}(\exp_p^{-1} Y) = 0. \]

If $[p]$ is a Ziezold mean of $X$ on $Q$ and optimal positioning is invariant, then $p$ is an extrinsic mean of $Y$ on $M$ and
\[ \mathbb{E}(\text{grad}(f_{ext})(\exp_p^{-1} Y)) = 0. \]

Proof of Theorem 4.7. The proof in case of Ziezold means is completely analogous to the following case of intrinsic means. With the hypotheses of Theorem 4.5, suppose that $L$ is a horizontal measurable lift of $\pi(U)$ guaranteed by Lemma 4.7 through an intrinsic mean $p \in M$ of the random element $Y$ on $M$ defined as in Lemma 4.8 with $[p] \in E^{d_q}(X)$. With the notation of Lemma 4.7 and its proof, if the assertion of the Theorem would be false, w.l.o.g. there would be a $q_j \in S^J$ with $gp_j \neq p_j$ for some $g \in I_p$ and $P\{Y \in M^J\} > 0$ for some $1 \leq j \leq J$ with
\[ M^J := \{\exp_p(tv) \in \exp_p(D) : v \in \exp_p^{-1}(L^J), t \geq 0\} \]
In particular, w.l.o.g. in the proof Lemma 4.7 we may choose an arbitrarily small $L^J_k$ around $p_j$ such that
\[ \int_{M^J_k} (\exp_p^{-1} Y - \exp_p^{-1}(gY)) dP_Y \neq 0. \]
with $M^J_k := \{\exp_p(tv) \in \exp_p(D) : v \in \exp_p^{-1}(L^J_k), t \geq 0\}$. Suppose that $L$ is obtained as in the proof of Lemma 4.7 by using $L^J_k$ and suppose that $L'$ is obtained from $L$ by replacing $L^J_k$ with $gL^J_k$. Then $L'$ is also a measurable horizontal lift in optimal position to $p$. Moreover with the lifts $Y'$ of $X$ to $L'$ and $Y$ of $X$ to $L$ guaranteed by Lemma 4.8 we have that
\[ 0 = \int_L \exp_p^{-1} Y dP_Y - \int_{L'} \exp_p^{-1} Y' dP_{Y'} \]
\[ = \int_{M^J_k} (\exp_p^{-1} Y - \exp_p^{-1}(dgY)) dP_Y \neq 0, \]
a contradiction to the above, completing the proof. \qed

Corollary 4.9. Suppose that a random pre-shape $Y$ is distributed on $M$ absolutely continuous w.r.t. Riemannian measure and supported by a tubular neighborhood that admits a slice through $p \in M$. Let $X = \pi \circ Y$ be the corresponding random shape. Then $p$ is regular if $[p]$ is an intrinsic mean of $X$, or if $[p]$ is a Ziezold mean, optimal positioning is invariant and [3] is valid.
5 Extrinsic Means for Kendall’s Shape Spaces

Let us recall the well known Veronese-Whitney embedding for Kendall’s planar shape spaces $\Sigma^k_2$. Identify $F^k_2$ with $\mathbb{C}^{k-1} \setminus \{0\}$ such that every landmark column corresponds to a complex number. This means in particular that $z \in \mathbb{C}^{k-1}$ is a complex row(!)-vector. With the Hermitian conjugate $a^* = \overline{(a_{jk})}$ of a complex matrix $a = (a_{jk})$ the pre-shape sphere $S^k_2$ is identified with $\{z \in \mathbb{C}^{k-1} : |z|^2 = 1\}$ on which $SO(2)$ identified with $S^1 = \{\lambda \in \mathbb{C} : |\lambda| = 1\}$ acts by complex scalar multiplication. Then the well known Hopf-Fibration mapping to complex projective space gives $\Sigma^k_2 = S^k_2/S^1 = \mathbb{CP}^{k-2}$. Moreover, denoting with $M(k-1,k-1,\mathbb{C})$ all complex $(k-1) \times (k-1)$ matrices, the Veronese-Whitney embedding is given by $z \in S^k_2/S^1 \mapsto \{a \in M(k-1,k-1,\mathbb{C}) : a^* = a\}$.

Remark 5.1. The Procrustes metric of $\Sigma^k_2$ is isometric with the Euclidean metric of $M(k-1,k-1,\mathbb{C})$ since we have $\langle z,w \rangle = \Re(z^*w)$ for $z,w \in S^k_2$ and hence, $d([z],[w]) = \sqrt{1 - z\overline{z}w\overline{w} = \|w^*w - z^*z\|/\sqrt{2}}$.

The idea of the Veronese-Whitney embedding can be transferred to the general case of shapes of arbitrary dimension $m \geq 2$. Even though the embedding given below is apt only for reflection shape space it can be applied to practical situations in similarity shape analysis whenever the geometrical objects considered have a common orientation. As above, the number $k$ of landmarks is essential and will be considered fixed throughout this section; the dimension $1 \leq m < k$, however, is lost in the embedding and needs to be retrieved by projection. To this end recall the (non-unique) embedding of $S^k_2$ in $S^m_2$ ($1 \leq j \leq m$) in [11] which gives rise to a unique and canonical embedding of $R\Sigma^m_2$ in $R\Sigma^k_2$. Moreover, consider the strata

$$(R\Sigma^m_2)_j := \{[x] \in R\Sigma^m_2 : \rank(x) = j\}, \quad (\Sigma^k_2)_j := \{[x] \in \Sigma^k_2 : \rank(x) = j\}$$

for $j = 1, \ldots, m$, each of which carries a canonical manifold structure; due to the above embedding, $(R\Sigma^m_2)_j$ can and will be identified with $(R\Sigma^k_2)_j$ such that

$$R\Sigma^k_2 = \bigcup_{j=1}^m (R\Sigma^k_2)_j.$$ 

At this point we note that $SO(m)$ is connected, while $O(m)$ is not; and the consequences for the respective manifold parts, i.e. points of maximal orbit type:

$$(\Sigma^k_2)^* = (\Sigma^k_2)^{m-1} \cup (\Sigma^k_2)^m,$$

$$(R\Sigma^k_2)^* = (R\Sigma^k_2)^m.$$
Similarly, we have a stratification

$$
\mathcal{P} := \left\{ a \in M(k-1,k-1) : a = a^T \geq 0, \text{tr}(a) = 1 \right\} = \bigcup_{j=1}^{k-1} \mathcal{P}^j
$$

of a bounded flat convex manifold $\mathcal{P}$ with non-flat unbounded manifolds

$$
\mathcal{P}^j := \{ a \in \mathcal{P} : \text{rank}(a) = j \} \ (j = 1, \ldots, k-1)
$$

all embedded in $M(k-1,k-1)$. The Schoenberg map $s : R\Sigma_m^k \to \mathcal{P}$ is then defined on each stratum by

$$
s|_{(R\Sigma_m^k)_j} : (R\Sigma_m^k)_j \to \mathcal{P}^j \quad x \mapsto x^T x.
$$

For $x \in S^k_j$ recall the tangent space decomposition $T_x S^k_j = T_x [x] \oplus H_x S^k_j$ into the vertical tangent space along the fiber $[x]$ and its orthogonal complement the horizontal tangent space. For $x \in (S^k_j)_j$ identify canonically (cf. Kendall et al. (1999, p. 109)):

$$
T_{[x]} (R\Sigma_j^k)^j \cong H_x S^k_j = \{ w \in M(j,k-1) : \text{tr}(wx^T) = 0, wx^T = xw^T \}.
$$

Then the assertion of the following Theorem condenses results of Bandulasiri and Patrangenaru (2005), cf. also Dryden et al. (2008).

**Theorem 5.2.** Each $s^j$ is a diffeomorphism with inverse $(s^j)^{-1}(a) = [(\sqrt{n}a^T)_j]$ where $a = u\lambda u^T$ with $u \in O(k-1)$, $\lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)$, and $0 = \lambda_{j+1} = \ldots = \lambda_{k-1}$ in case of $j < k-1$. Here, $(a)_j$ denotes the matrix obtained from taking only the first $j$ rows from $a$. For $x \in S^k_j$ and $w \in H_x S^k_j \cong T_{[x]} (R\Sigma_j^k)^j$ the derivative is given by

$$
d(s^j)|_{[x]}w = x^T w + w^T x.
$$

**Remark 5.3.** In contrast to the Vernose-Whitney embedding, the Schoenberg embedding is not isometric as the example of

$$
x = \begin{pmatrix} \cos \phi & 0 \\ 0 & \sin \phi \end{pmatrix}, \quad w_1 = \begin{pmatrix} \sin \phi & 0 \\ 0 & -\cos \phi \end{pmatrix}, \quad w_2 = \begin{pmatrix} 0 & \cos \phi \\ \sin \phi & 0 \end{pmatrix},
$$
teaches:

$$
\|x^T w_1 + w_1^T x\| = \sqrt{2}|\cos \phi \sin \phi|, \quad \|x^T w_2 + w_2^T x\| = \sqrt{2}.
$$

Since $\mathcal{P}$ is bounded, convex and Euclidean, the classical expectation $E(X^T X) \in \mathcal{P}^j$ for some $1 \leq j \leq k-1$ of the Schoenberg image $X^T X$ of an arbitrary random reflection shape $[X] \in R\Sigma_m^k$ is well defined. Then we have at once the following relation between rank of Euclidean mean and increasing sample size.
Theorem 5.4. Suppose that a random reflection shape $[X] \in R^{(k-1)}$ is distributed absolutely continuous w.r.t. the projection of the spherical measure on $S^k_m$. Then

$$E(X^T X) \in P^{k-1}$$

for every i.i.d. sample $X_1, \ldots, X_n \sim X$ if $j \leq nm < j + 1$ for $nm < k - 1$ and $j = k - 1$ for $nm \geq k - 1$.

Hence, in statistical settings involving a higher number of landmarks, a sufficiently well-behaved projection of a high rank Euclidean mean onto lower rank $P^r \cong (S^k_m)^r$, usually $m = r$, is to be employed, giving at once a mean shape satisfying strong consistency and a CLT. Here, unlike to intrinsic or Procrustes analysis, the dimension $r$ chosen is crucial for the dimensionality of the mean obtained.

The orthogonal projection

$$\phi^r : \bigcup_{i=r}^{k-1} P^i \rightarrow P^r$$

$$a \mapsto \arg\min_{b \in P^r} \text{tr}\left( (a - b)^2 \right)$$

giving the set of extrinsic Schoenberg means has been computed by Bhattacharya [2008].

Theorem 5.5. For $1 \leq r \leq k - 1$, $a = u\lambda u^T \in P$ with $u \in O(k - 1)$, $\lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)$, $\lambda_1 \geq \ldots \geq \lambda_{k-1}$ and $\lambda_r > 0$ the orthogonal projection onto $P^r$ is given by

$$\phi^r(a) = u\mu u^T$$

with $\mu = \text{diag}(\mu_1, \ldots, \mu_r, 0, \ldots, 0)$,

$$\mu_i = \lambda_i + \frac{1}{r} - \lambda_r (i = 1, \ldots, r)$$
and $\bar{\lambda}_r = \frac{1}{r} \sum_{i=1}^{r} \lambda_i \leq \frac{1}{r}$ which is uniquely determined if and only if $\lambda_r > \lambda_{r+1}$.

With the notation of Theorem 5.5, a non-orthogonal central projection $\psi^r(a) = u \nu u^T$ equally well and uniquely determined has been proposed by Dryden et al. (2008) with $\nu = \text{diag}(\nu_1, \ldots, \nu_r, 0, \ldots, 0)$,

$$\nu_i = \frac{\lambda_i}{r \bar{\lambda}_r} \quad (i = 1, \ldots, r).$$

Orthogonal and central projection are depicted in Figure 5.

6 Local Effects of Curvature

In this section we assume that a manifold stratum $M$ supporting a random element $X$ is isometrically embedded in a Euclidean space $\mathbb{R}^D$ of dimension $D > 0$. With the orthogonal projection $\Phi : \mathbb{R}^D \to M$ from Section 3 and the Riemann exponential $\exp_p$ of $M$ at $p$ we have the

intrinsinc tangent space coordinate $\exp_p^{-1} X$ and the residual tangent space coordinate $d\Phi_p(X - p)$,

respectively, of $X$ at $p$, if existent.

6.1 Finite Power of Tests and Tangent Space Coordinates

With the above setup, assume that $\mu \in M$ is a unique mean of $X$. If $c \in \mathbb{R}^D$ is the center of the osculatory circle touching the geodesic segment in $M$ from $X$ to $\mu$ at $\mu$ with radius $r$, and if $X_r$ is the orthogonal projection of $X$ to that circle, then $X = X_r + O(\|X - \mu\|^3)$. Moreover, with

$$\cos \alpha = \left\langle \frac{X - c}{\|X - c\|}, \frac{\mu - c}{r} \right\rangle = \frac{1}{r^2} (X_r - c, \mu - c) + O(\|X - \mu\|^3)$$

we have the residual tangent space coordinate

$$v = X - c - \frac{\mu - c}{r} \|X - c\| \cos \alpha = X_r - c - (\mu - c) \cos \alpha + O(\|X - \mu\|^3)$$

having squared length $\|v\|^2 = r^2 \sin \alpha^2 + O(\|X - \mu\|^3)$. By isometry of the embedding, the intrinsic tangent space coordinate is given by

$$\exp_{\mu} X = \frac{r \alpha}{\|v\|} v + O(\|X - \mu\|^3).$$

With the component

$$\nu = \mu - c - \|X - c\| \frac{\mu - c}{r} \cos \alpha = (\mu - c)(1 - \cos \alpha) + O(\|X - \mu\|^3)$$

$$= \frac{1}{r^2} (X_r - c, \mu - c) + O(\|X - \mu\|^3)$$

we have the residual tangent space coordinate

$$v = X - c - \frac{\mu - c}{r} \|X - c\| \cos \alpha = X_r - c - (\mu - c) \cos \alpha + O(\|X - \mu\|^3)$$

having squared length $\|v\|^2 = r^2 \sin \alpha^2 + O(\|X - \mu\|^3)$. By isometry of the embedding, the intrinsic tangent space coordinate is given by

$$\exp_{\mu} X = \frac{r \alpha}{\|v\|} v + O(\|X - \mu\|^3).$$

With the component

$$\nu = \mu - c - \|X - c\| \frac{\mu - c}{r} \cos \alpha = (\mu - c)(1 - \cos \alpha) + O(\|X - \mu\|^3)$$

$$= \frac{1}{r^2} (X_r - c, \mu - c) + O(\|X - \mu\|^3)$$

$$= \frac{1}{r^2} (X_r - c, \mu - c) + O(\|X - \mu\|^3)$$

we have the residual tangent space coordinate

$$v = X - c - \frac{\mu - c}{r} \|X - c\| \cos \alpha = X_r - c - (\mu - c) \cos \alpha + O(\|X - \mu\|^3)$$

having squared length $\|v\|^2 = r^2 \sin \alpha^2 + O(\|X - \mu\|^3)$. By isometry of the embedding, the intrinsic tangent space coordinate is given by

$$\exp_{\mu} X = \frac{r \alpha}{\|v\|} v + O(\|X - \mu\|^3).$$

With the component

$$\nu = \mu - c - \|X - c\| \frac{\mu - c}{r} \cos \alpha = (\mu - c)(1 - \cos \alpha) + O(\|X - \mu\|^3)$$

$$= \frac{1}{r^2} (X_r - c, \mu - c) + O(\|X - \mu\|^3)$$
of $X$ normal to the mentioned geodesic segment of squared length $\|\nu\|^2 = r^2(1 - \cos^2 \alpha) + O(||X - \mu||^3)$ we obtain

$$\| \exp_{\mu} X \|^2 = \|v\|^2 + \|\nu\|^2 + O(||X - \mu||^3),$$

since

$$(1 - \cos^2 \alpha) + \sin^2 \alpha = 2(1 - \cos^2 \alpha) = \alpha^2 + 2\frac{\alpha^4}{4!} + \cdots$$

and $\alpha = O(||X - \mu||)$. In consequence we have

**Remark 6.1.** In approximation, the variation of intrinsic tangent space coordinates is the sum of the variation $\|v\|^2$ of residual tangent space coordinates and the variation normal to it. In particular, for spheres

$$\| \exp_{\mu} X \|^2 \geq \|v\|^2 + \|\nu\|^2.$$

Since the variation in normal space is irrelevant for a two-sample test for equality of means, say, a higher power for tests based on intrinsic means can be expected when solely residual tangent space coordinates obtained from an isometric embedding are used rather than intrinsic tangent space coordinates.

Note that the natural tangent space coordinates for Ziezold means are residual.

A simulated classification example in Section 7 illustrates this slight effect.

### 6.2 The 1 : 3 - Property for Spherical and Kendall Shape Means

In this section $M = S^{D-1} \subset \mathbb{R}^D$ is the $(D - 1)$-dimensional unit-hypersphere embedded isometrically in Euclidean $D$-dimensional space. The orthogonal projection $\Phi : \mathbb{R}^D \rightarrow S^{D-1} : p \rightarrow \frac{p}{\|p\|}$ is well defined except for the origin $p = 0$, and the normal space at $p \in S^{D-1}$ is spanned by $p$ itself. In consequence, a random point $X$ on $S^{D-1}$ has

$$d\Phi_p(X - p) = X - p \cos \alpha, \quad \exp_p(X) = \frac{\alpha}{\sin \alpha} d\Phi_p(X - p)$$

as residual and intrinsic, resp., tangent space coordinate at $-X \neq p \in S^{D-1}$ where $\cos \alpha = \langle X, p \rangle$.

**Remark 6.2.** An adaption (i.e. multiplying by the respective $\sin \alpha$ in every iteration step) of the algorithm for intrinsic means in [Huckemann and Ziezold (2006), Section 5.4] gives at once an algorithm converging usually quickly to one of the two sample residual means.

**Theorem 6.3.** If $X$ is contained in a closed half sphere with non-zero probability in its interior, it has a unique intrinsic mean which is assumed in the interior of that half sphere.

17
Proof. Below, we show that every intrinsic mean necessarily lies within the interior of the half sphere. Then, Kendall (1990, Theorem 7.3) yields uniqueness. W.l.o.g. let \( X = (\sin \phi, x_2, \ldots, x_n) \) such that \( \mathbb{P}\{\sin \phi < 0\} = 0 < \mathbb{P}\{\sin \phi > 0\} \) and assume that \( p = (\sin \psi, p_2, \ldots, p_n) \in S^{D-1} \) is an intrinsic mean. Moreover let \( p' = (\sin(|\psi|), p_2, \ldots, p_n) \). Since
\[
E\left( \| \exp_p(X) \|^2 \right) = E\left( \arccos^2 \langle p, X \rangle \right)
\]
\[
= E\left( \arccos^2 \left( \sin \phi \sin \psi + \sum_{j=2}^{n} p_j x_j \right) \right)
\]
\[
\leq E\left( \| \exp_{p'}(X) \|^2 \right)
\]
with equality if and only if \(|\psi| = \psi\), this can only happen for \( \psi \geq 0 \). Now, suppose that \( p = (0, p_2, \ldots, p_n) \) is an intrinsic mean. For deterministic \( \psi \geq 0 \) consider \( p(\psi) = (\sin \psi, p_1 \cos \psi, \ldots, p_n \cos \psi) \). Then
\[
E\left( \| \exp_{p(\psi)}(X) \|^2 \right) = E\left( \arccos^2 \left( \sin \psi \sin \phi + \cos \phi \sum_{j=2}^{n} p_j x_j \right) \right)
\]
\[
= E\left( \| \exp_p(X) \|^2 \right) - C_1 \psi + O(\psi^2)
\]
with \( C_1 > 0 \) since \( \mathbb{P}\{\sin \phi > 0\} > 0 \). In consequence, \( p \) cannot be an intrinsic mean. Hence, we have shown that every intrinsic mean is contained in the interior of the half sphere.

Remark 6.4. For the special case of spheres, this extends a result of H. Le, asserting a unique intrinsic mean on general Riemannian manifolds, if among others, the support of \( X \) is contained in a geodesic quarter-ball, see Le (2001, 2004). H. Le’s result is an extension of Karcher (1977), asserting uniqueness of intrinsic means in geodesic balls if among others, \( X \) is supported in a geodesic quarter ball. Intrinsic means restricted to geodesic balls are often called Karcher means. As mentioned in the above proof, Kendall (1990, Theorem 7.3) extended Karcher’s result to obtain uniqueness of Karcher means, if among others, the support of \( X \) is contained in a half ball. In view of Theorem 6.3, one might expect to extend Le’s result on uniqueness of intrinsic means on the entire manifold accordingly, to random elements contained in a geodesic half ball.

The following Theorem characterizes the three spherical means.

Theorem 6.5. Let \( X \) be a random point on \( S^{D-1} \). Then \( x^{(e)} \in S^{D-1} \) is the unique extrinsic mean if and only if the Euclidean mean \( \mathbb{E}(X) = \int_{S^{D-1}} X \, dP_X \) is non-zero. If the following right hand sides are non-zero, then there are suitable \( \lambda^{(e)} = \| \mathbb{E}(X) \| > 0 \), \( \lambda^{(r)} > 0 \) and \( \lambda^{(i)} > 0 \) such that
\[
\lambda^{(e)} x^{(e)} = \mathbb{E}(X),
\]

every residual mean \( x^{(r)} \in S^{D-1} \) satisfies
\[
\lambda^{(r)} x^{(r)} = \mathbb{E}\left( (X, x^{(r)}) X \right),
\]

18
and every intrinsic mean \( x^{(i)} \in S^{D-1} \) satisfies
\[
\lambda^{(i)} x^{(i)} = E \left( \frac{\arccos(\langle X, x^{(i)} \rangle)}{\sqrt{1 - \langle X, x^{(i)} \rangle^2}} X \right).
\]

In the last case we additionally require that \( E \left( \frac{\arccos(\langle X, x^{(i)} \rangle)}{\sqrt{1 - \langle X, x^{(i)} \rangle^2}} \right) > 0 \) which is in particular the case if \( X \) is contained in a closed half sphere with non-zero probability in the interior.

**Proof.** The assertions for the extrinsic mean are well known from [Hendriks et al. (1996)]. The second assertion for residual means follows from minimization of
\[
\int_{S^{D-1}} \| p - \langle p, x \rangle x \|^2 dP_X(p) = 1 - \int_{S^{D-1}} \langle p, x \rangle^2 dP_X(p)
\]
with respect to \( x \in \mathbb{R}^D \) under the constraining condition \( \| x \| = 1 \). Using a Lagrange ansatz this leads to the necessary condition
\[
\int_{S^{D-1}} \langle p, x \rangle p dP_X(p) = \lambda x
\]
with a Lagrange multiplier \( \lambda \) of value \( E(\langle X, x \rangle^2) \) which is positive unless \( X \) is supported by the hypersphere orthogonal to \( x \). In that case, by Theorem 3.3, \( x \) cannot be a residual mean of \( X \), as every residual mean is as well contained in that hypersphere. Hence, we have \( \lambda > 0 \). The same method applied to
\[
\int_{S^{D-1}} \| \exp^{-1}(p) \|^2 dP_X(p) = \int_{S^{D-1}} \arccos^2(\langle p, x \rangle) dP_X(p)
\]
taking into account Theorem 6.3 yields the third assertion on the intrinsic mean. \( \square \)

In particular, residual means are eigenvectors to the largest eigenvalue of the matrix \( E(XX^T) \). As such, they rather reflect the mode then the classical mean of a distribution:

**Example 6.6.** Consider \( \gamma \in (0, \pi) \) and a random variable \( X \) on the unit circle \( \{ e^{i \theta} : \theta \in [0, 2\pi] \} \) which takes the value 1 with probability 2/3 and \( e^{i \gamma} \) with probability 1/3. Then, explicit computation gives the unique intrinsic and extrinsic mean as well as the two residual means
\[
x^{(i)} = e^{i \frac{\pi}{2}}, \quad x^{(e)} = e^{i \arctan \frac{\sin \gamma}{\cos \gamma}}, \quad x^{(r)} = \pm e^{i \frac{\pi}{4} \arctan \frac{\sin(2 \gamma)}{\cos(2 \gamma)}}.
\]

Figure 2 shows the case \( \gamma = \frac{\pi}{4} \).

In contrast to Figure 2 one may assume in many practical applications that the mutual proximities of the unique intrinsic mean \( x^{(i)} \), the unique extrinsic mean \( x^{(e)} \) and the unique residual mean \( x^{(r)} \) closer to \( x^{(e)} \) are rather small,
namely of the same order as the squared proximity of the modulus $\|E(X)\|$ of the Euclidean mean to 1, cf. Table 1. We will use the following condition

$$
\|x^{(e)} - x^{(r_0)}\|, \quad \|x^{(e)} - x^{(i)}\| = O\left((1 - \|E(X)\|)^2\right) 
$$

with the concentration parameter $1 - \|E(X)\|$.

**Corollary 6.7.** Under condition (5), if all three means are unique, then the great circular segment between the residual $x^{(r_0)}$ mean closer to the extrinsic mean $x^{(e)}$ and the intrinsic mean $x^{(i)}$ is divided by the extrinsic mean in approximation by the ratio $1 : 3$:

$$
x^{(r_0)} = \frac{\|E(X)\|}{\lambda^{(r_0)}} \left(x^{(e)} - \frac{E((X - x^{(e)}, X) X)}{\|E(X)\|} + O\left((1 - \|E(X)\|)^2\right)\right)
$$

$$
x^{(i)} = \frac{\|E(X)\|}{\lambda^{(i)}} \left(x^{(e)} + \frac{1}{3} \frac{E((X - x^{(e)}, X) X)}{\|E(X)\|} + O\left((1 - \|E(X)\|)^2\right)\right)
$$

with $\lambda^{(i)}$ and $\lambda^{(r_0)}$ from Theorem 6.5

**Proof.** For any $x, p \in S^{D-1}$ decompose $p - x = p - \langle x, p \rangle x - z(x, p)x$ with $z(x, p) = 1 - \langle x, p \rangle$, the length of the part of $p$ normal to the tangent space at $x$. Note that $E\left(z(x^{(e)}, X)\right) = 1 - \|E(X)\|$. Now, under condition (5), verify the first assertion using Theorem 6.5

$$
x^{(r_0)} = \frac{1}{\lambda^{(r_0)}} \left(E(X) - E\left(z(x^{(r_0)}, X)X\right)\right).
$$

On the other hand since

$$
\frac{\arccos(1 - z)}{\sqrt{1 - (1 - z)^2}} = 1 + \frac{1}{3} z + \frac{2}{15} z^2 + \ldots
$$
we obtain with the same argument the second assertion

\[
x^{(i)} = \frac{1}{\lambda^{(i)}} \mathbb{E} \left( \frac{\arccos(X, x^{(i)})}{\sqrt{1 - (X, x^{(i)})^2}} X \right)
\]

\[
= \frac{1}{\lambda^{(i)}} \left( \mathbb{E}(X) + \frac{1}{3} \mathbb{E} \left( z(x^{(i), X}) X \right) + \frac{2}{15} \mathbb{E} \left( z(x^{(i), X})^2 X \right) + \ldots \right)
\]

\[
= \frac{\|\mathbb{E}(X)\|}{\lambda^{(i)}} \left( x^{(e)} + \frac{1}{3\|\mathbb{E}(X)\|} \mathbb{E} \left( z(x^{(e), X}) X \right) + O((1 - \|\mathbb{E}(X)\|)^2) \right).
\]

\[\square\]

**Remark 6.8.** The tangent vector defining the great circle approximately connecting the three means is obtained from correcting with the expected normal component of any of the means. As numerical experiments show, this great circle is different from the first principal component geodesic as defined in [Huckemann and Ziezold (2006)](Huckemann:2006).

Recall the following connection between intrinsic and extrinsic spherical versus intrinsic and Ziezold shape means, respectively, cf. Lemmas 4.1 and 4.8. It is easy to see the corresponding connection for residual versus Procrustes means.

**Remark 6.9.** Suppose that a random shape \(X\) on \(\Sigma^k_m\) is supported by \(R \subset \Sigma^k_m\) admitting a horizontal measurable lift \(L \subset S^k_m\) in optimal position to \(p \in S^k_m\). Define the random variable \(Y\) on \(S^k_m\) by \(\pi \circ Y = X\). Then we have that

- if \([p]\) is an intrinsic mean of \(X\) then \(p\) is an intrinsic mean of \(Y\),
- if \([p]\) is a Procrustes mean of \(X\) then \(p\) is a residual mean of \(Y\),
- if \([p]\) is a Ziezold mean of \(X\) then \(p\) is an extrinsic mean of \(Y\)

In consequence, Corollary 6.7 extends at once to Kendall’s shape spaces.

**Corollary 6.10.** Suppose that a random shape \(X\) on \(\Sigma^k_m\) with unique intrinsic mean \(\mu^{(i)}\), unique Ziezold mean \(\mu^{(z)}\) and unique Procrustes mean \(\mu^{(p_0)}\) closer to \(\mu^{(i)}\) is supported by \(R \subset \Sigma^k_m\) admitting a horizontal measurable lift \(L \subset S^k_m\) in optimal position to \(\mu^{(z)} \in S^k_m\). If the means are sufficiently close to each other in the sense of

\[
d_{\Sigma^k_m}(\mu^{(z)} - \mu^{(p_0)}), \quad d_{S^k_m}(\mu^{(z)} - \mu^{(i)}) = O((1 - \|\mathbb{E}(Y)\|)^2)
\]

with the random pre-shape \(Y\) on \(L\) defined by \(X = \pi \circ Y\), then the generalized geodesic segment between \(\mu^{(i)}\) and \(\mu^{(p_0)}\) is approximately divided by \(\mu^{(z)}\) by the ratio 1 : 3 with an error of order \(O((1 - \|\mathbb{E}(Y)\|)^2)\).
7 Examples: Exemplary Datasets and Simulations

7.1 The 1 : 3 property

In the first example we illustrate Corollary 6.11 on the basis of four data sets:

**poplar leaves:** contains 104 quadrangular planar shapes extracted from poplar leaves in a joint collaboration with Institute for Forest Biometry and Informatics at the University of Göttingen, cf. Huckemann et al. (2009).

**digits ‘3’:** contains 30 planar shapes with 13 landmarks each, extracted from handwritten digits ‘3’, cf. Dryden and Mardia (1998, p. 318).

**macaque skulls:** contains three-dimensional shapes with 7 landmarks each, of 18 macaque skulls, cf. Dryden and Mardia (1998, p. 16).

**iron age brooches:** contains 28 three-dimensional tetrahedral shapes of iron age brooches, cf. Small (1996, Section 3.5).

![Shape means for four typical data sets](image)

Figure 3: Depicting shape means for four typical data sets: intrinsic (star), Ziezold (circle) and Procrustes (diamond) projected to the tangent space at the intrinsic mean. The cross divides the generalized geodesic segment joining the intrinsic with the Procrustes mean by the ratio 1 : 3.
Table 1: Mutual shape distances between intrinsic mean \( \mu^{(i)} \), Ziezold mean \( \mu^{(z)} \) and Procrustes mean \( \mu^{(p_0)} \) closer to the Ziezold mean for various data sets.
Right column: the squared distance between modulus of Euclidean mean and 1, cf. Corollary 6.10.

As clearly visible from Figure 3 and Table 1, the approximation of Corollary 6.10 for two- and three-dimensional shapes is highly accurate for data of little dispersion (the macaque skull data) and still fairly accurate for highly dispersed data (the digits ’3’ data).

![Figure 4](image-url)

Figure 4: A data set of three planar triangles (top row) with its corresponding intrinsic mean (bottom left), Ziezold mean (bottom center) and Procrustes mean (bottom right).
Figure 5: Planar triangles $q_1 = x \cos \beta - w_2 \sin \beta$, $q_2 = x \cos \beta - w_2 \sin \beta$ and $q = x \cos \beta' + w_1 \sin \beta'$ with $x, w_1, w_2$ from Remark 5.3, $\phi = 0.05$, $\beta = 0.3 = \beta'$ (top row). Intrinsic means (middle row) of sample $(q_1, q_2)$ (left) and $(q_1, q_2, q)$ (right). Schoenberg means (bottom row) of sample $(q_1, q_2)$ (left) and $(q_1, q_2, q)$ (right).

7.2 “Blindness” of Procrustes and Schoenberg Means

In the second example we illustrate an effect of “blindness to data” of Procrustes means and Schoenberg means. The former blindness is due to the affinity of the Procrustes mean to the mode in conjunction with curvature, the latter is due to non-isometry of the Schoenberg embedding. While the former effect occurs only for some highly dispersed data when the analog of condition (6) is violated, the latter effect is local in nature and may occur for concentrated data as well.

Example 7.1. Reenacting the situation of Example 6.6 and Figure 2, the shapes of the triangles $P$ and $Q$ in Figure 4 are almost maximally remote. Since the
mode $P$ is assumed twice and $Q$ only once, the Procrustes mean is nearly blind to $Q$. In case of

$$P = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 1 & 1 & -2 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{3}{\sqrt{2}} \end{pmatrix}$$

the Procrustes mean shape of the sample $P, P, Q$ is the one-dimensional $P$ because of blindness to the two-dimensional $Q$.

Let us record this fact.

**Remark 7.2.** The Procrustes mean of a random shape assuming both regular and degenerate shapes with non-zero probability may be degenerate.

Even though Schoenberg means have been introduced to tackle 3D shapes, the effect of "blindness" can be well illustrated already for 2D. To this end consider $x = x(\phi)$, $w_1 = w_1(\phi)$ and $w_2 = w_2(\phi)$ as introduced in Remark 5.3. Along the horizontal geodesic through $x$ with initial velocity $w_2$ we pick two points $q_1 = x \cos \beta + w_2 \sin \beta$ and $q_2 = x \cos \beta - w_2 \sin \beta$. On the orthogonal horizontal geodesic through $x$ with initial velocity $w_1$ pick $q = x \cos \beta' + w_1 \sin \beta'$. Recall from Remark 5.3 that along that geodesic the derivative of the Schoenberg embedding can be made arbitrarily small for $\phi$ near 0. Indeed, Figure 5 illustrates that for small $\phi$, the Schoenberg mean is nearly unchanged if the triangle $q$ is added to the sample $q_1, q_2$. The corresponding intrinsic means, however, are sensitive to the sample’s expansions.

![Figure 6: cube (left) and pyramid (right) for classification.](image)

**7.3 Classification Power of a Test**

In the ultimate example we illustrate the consequences of the choice of tangent space coordinates and the effect of the tendency of the Schoenberg mean to increase dimension by a classification simulation. To this end we apply a Hotelling $T^2$-test to discriminate the shapes of 10 noisy samples of regular unit cubes from the shapes of 10 noisy samples of pyramids with top section chopped off, each
with 8 landmarks, given by the following configuration matrix

$$
\begin{pmatrix}
0 & 1 & \frac{1+\varepsilon}{2} & \frac{1-\varepsilon}{2} & 0 & 1 & \frac{1+\varepsilon}{2} & \frac{1-\varepsilon}{2} \\
0 & 0 & \frac{1+\varepsilon}{2} & \frac{1-\varepsilon}{2} & 1 & 1 & \frac{1+\varepsilon}{2} & \frac{1-\varepsilon}{2} \\
0 & 0 & \varepsilon & \varepsilon & 0 & 0 & \varepsilon & \varepsilon
\end{pmatrix}
$$

(cf. Figure 6) determined by \( \varepsilon > 0 \). In the simulation, independent Gaussian noise with variance \( \sigma^2 > 0 \) is added to each landmark measurement. Table 2 gives the number of correct classifications for 1,000 simulations for given \( \alpha, \varepsilon \) and significance level.

| \( \sigma \) | \( \varepsilon \) | level | intrinsic mean with residual tangent space coordinates | Ziezold mean | Procrustes mean | Schoenberg mean |
|---|---|---|---|---|---|---|
| 0.35 | 0.05 | 0.1 | 522 | 542 | 538 | 631 | 442 |
| 0.3 | 0.1 | 0.1 | 558 | 583 | 581 | 575 | 483 |
| 0.2 | 0.2 | 0.05 | 556 | 575 | 574 | 575 | 512 |
| 0.1 | 0.3 | 0.01 | 359 | 369 | 369 | 368 | 366 |
| 0.05 | 0.35 | 0.01 | 764 | 780 | 780 | 780 | 809 |

Table 2: Number of correct classifications within 1,000 simulations each of 10 unit-cubes and pyramids determined by \( \varepsilon \) (which gives the height), where each landmark is independently corrupted by Gaussian noise of variance \( \sigma^2 \), via a Hotelling \( T^2 \)-test for equality of means to the given significance level.

As visible from Table 2, discriminating nearly flat pyramids (\( \varepsilon = 0.05 \)) from cubes is achieved much better by employing intrinsic, Ziezold or Procrustes means rather than Schoenberg means. This finding is in concord with Theorem 5.4: samples of size 10 of three-dimensional configurations yield Euclidean means a.s. in \( \mathcal{P}^7 \) which are projected to \( \mathcal{P}^3 \) to obtain Schoenberg means in \( \Sigma_3^8 \). In consequence, Schoenberg means of nearly two-dimensional pyramids are essentially three dimensional. With increased height of the pyramid (\( \varepsilon = 0.35 \)), i.e. for more pronounced third dimension and increased proximity to the unit cube), all means perform almost equally well, with a tendency of the Schoenberg mean to eventually outperform the others. Moreover in any case, intrinsic means with intrinsic tangent space coordinates behave much poorer in view of shape discrimination than intrinsic means with residual tangent space coordinates, cf. Remark 6.1. The latter (intrinsic means with residual tangent space coordinates) are better or equally good as Ziezold and Procrustes means (which naturally use residual tangent space coordinates).

| intrinsic mean | Ziezold mean | Procrustes mean | Schoenberg mean |
|---|---|---|---|
| 235.167 | 182.335 | 225.982 | 35.595 |

Table 3: Average time in seconds for computation of 1,000 means of sample size 20.

In conclusion we record the time for mean computation in Table 3. While
Ziezold means compute in approximately $3/4$ of the computational time for intrinsic means, Schoenberg means are obtained approximately 5 times faster.

Note that we have included inference based on Procrustes means for illustration, even though no stability result is available and hence at this point, it cannot be theoretically justified that the CLT holds for Procrustes means as well.

8 Discussion

By establishing stability results for intrinsic and Ziezold means on the manifold part of a shape space, a gap in asymptotic theory for general non-manifold shape spaces could be closed, now allowing for multi-sample tests of equality of intrinsic means and Ziezold means. A similar stability assertion in general is false for Procrustes means. Note that the argument applied to intrinsic and Ziezold means fails for Procrustes means, since in contrast to (3) the sum of Procrustes residuals is in general non-zero. The findings on dimensionality condense to

- Procrustes means may decrease dimension,
- intrinsic and Ziezold means preserve dimension,
- Schoenberg means tend to increase dimension.

Due to the proximity of Ziezold and intrinsic means on Kendall’s shape spaces in most practical applications, taking into account that the former are computationally easier accessible (optimally positioning and Euclidean averaging in every iteration step) than intrinsic means (optimally positioning and weighted averaging in every iteration step), in practical applications Ziezold means, may be preferred over intrinsic means. They may be even more preferred over intrinsic means, since Ziezold means naturally come with residual tangent space coordinates which may allow in case of intrinsic means for a slightly higher finite power of tests than intrinsic tangent space coordinates.

Computationally much faster (not relying on iteration at all) are Schoenberg means which are available for Kendall’s reflection shape spaces. As a drawback, however, Schoneberg means, seem less sensitive for dimensionality of configurations considered than intrinsic or Ziezold means. In consequence, multi-sample test based on Schoenberg means may have a considerably lower power than when based on intrinsic or Ziezold means.

We note that Ziezold means may be defined for the shape spaces of planar curves introduced by Zahn and Roskies (1972), which are currently very popular e.g. Klassen et al. (2004) or Schmidt et al. (2006). Employing Ziezold means there, a computational advantage greater than found here can be expected since computation of iterates of intrinsic means involve computations of geodesics which themselves can only be found iteratively.
Acknowledgment

The author would like to thank Alexander Lytchak for helpful advice on differential geometric issues. Also, the author gratefully acknowledges support by DFG grant MU 1230/10-1 and GRK 1023.

References

Bandulasiri, A., Patrangenaru, V., 2005. Algorithms for nonparametric inference on shape manifolds.

Bhattacharya, A., 2008. Statistical analysis on manifolds: A nonparametric approach for inference on shape spaces. To appear.

Bhattacharya, R. N., Patrangenaru, V., 2003. Large sample theory of intrinsic and extrinsic sample means on manifolds I. Ann. Statist. 31 (1), 1–29.

Bhattacharya, R. N., Patrangenaru, V., 2005. Large sample theory of intrinsic and extrinsic sample means on manifolds II. Ann. Statist. 33 (3), 1225–1259.

Blum, H., Nagel, R. N., 1978. Shape description using weighted symmetric axis features. Pattern Recognition 10 (3), 167–180.

Bredon, G. E., 1972. Introduction to Compact Transformation Groups. Vol. 46 of Pure and Applied Mathematics. Academic Press.

Choquet, G., 1954. Theory of capacities. Ann. Inst. Fourier 5, 131–295.

Dryden, I. L., Kume, A., Le, H., Wood, A. T. A., 2008. A multidimensional scaling approach to shape analysis. To appear.

Dryden, I. L., Mardia, K. V., 1998. Statistical Shape Analysis. Wiley, Chichester.

Fréchet, M., 1948. Les éléments aléatoires de nature quelconque dans un espace distancié. Ann. Inst. H. Poincaré 10 (4), 215–310.

Gower, J. C., 1975. Generalized Procrustes analysis. Psychometrika 40, 33–51.

Hendriks, H., 1991. A Cramér-Rao type lower bound for estimators with values in a manifold. Journal of Multivariate Analysis 38, 245–261.

Hendriks, H., Landsman, Z., 1996. Asymptotic behaviour of sample mean location for manifolds. Statistics & Probability Letters 26, 169–178.

Hendriks, H., Landsman, Z., 1998. Mean location and sample mean location on manifolds: asymptotics, tests, confidence regions. Journal of Multivariate Analysis 67, 227–243.
Hendriks, H., Landsman, Z., Ruyngaart, F., 1996. Asymptotic behaviour of sample mean direction for spheres. Journal of Multivariate Analysis 59, 141–152.

Hobolth, A., Kent, J., Dryden, I., 2002. On the relation between edge and vertex modelling in shape analysis. Scandinavian Journal of Statistics 29 (3), 355–374.

Hotz, T., Huckemann, S., Gaffrey, D., Munk, A., Sloboda, B., 2010. Shape spaces for pre-aligning star-shaped objects in studying the growth of plants. Journal of the Royal Statistical Society, Series C 59 (1), 127–143.

Huckemann, S., Hotz, T., Munk, A., 2009. Intrinsic MANOVA for Riemannian manifolds with an application to Kendall’s space of planar shapes. IEEE Transactions on Pattern Analysis and Machine Intelligence. To appear.

Huckemann, S., Ziezold, H., 2006. Principal component analysis for Riemannian manifolds with an application to triangular shape spaces. Adv. Appl. Prob. (SGSA) 38 (2), 299–319.

Jupp, P. E., 1988. Residuals for directional data. J. Appl. Statist. 15 (2), 137–147.

Karcher, H., 1977. Riemannian center of mass and mollifier smoothing. Communications on Pure and Applied Mathematics XXX, 509–541.

Kendall, D., 1974. Foundations of a theory of random sets. Stochastic Geom., Tribute Memory Rollo Davidson, 322–376 (1974).

Kendall, D. G., 1984. Shape manifolds, Procrustean metrics and complex projective spaces. Bull. Lond. Math. Soc. 16 (2), 81–121.

Kendall, D. G., Barden, D., Carne, T. K., Le, H., 1999. Shape and Shape Theory. Wiley, Chichester.

Kendall, W. S., 1990. Probability, convexity, and harmonic maps with small image I: Uniqueness and fine existence. Proc. London Math. Soc. 61, 371–406.

Klassen, E., Srivastava, A., Mio, W., Joshi, S., Mar. 2004. Analysis on planar shapes using geodesic paths on shape spaces. IEEE Transactions on Pattern Analysis and Machine Intelligence 26 (3), 372–383.

Kobayashi, S., Nomizu, K., 1969. Foundations of Differential Geometry. Vol. II. Wiley, Chichester.

Krim, H., Yezzi, A. J. J. E., 2006. Statistics and Analysis of Shapes. Modeling and Simulation in Science, Engineering and Technology. Birkhäuser, Boston.

Le, H., Jun. 2001. Locating Fréchet means with an application to shape spaces. Adv. Appl. Prob. (SGSA) 33 (2), 324–338.
Le, H., 2004. Estimation of Riemannian barycenters. LMS Journal of Computation and Mathematics 7, 193–200.

Mardia, K., Patrangenaru, V., 2001. On affine and projective shape data analysis. Functional and Spatial Data Analysis, Proceedings of the 20th LASR Workshop (Eds: K.V. Mardia and R.G. Aykroyd), 39–45.

Mardia, K., Patrangenaru, V., 2005. Directions and projective shapes. Ann. Statist. 33, 1666–1699.

Matheron, G., 1975. Random sets and integral geometry. Wiley Series in Probability and Mathematical Statistics. New York.

Mosimann, J. E., 1970. Size allometry: Size and shape variables with characterizations of the lognormal and generalized gamma distributions. Journal of the American Statistical Association 65 (330), 930–945.

Munk, A., Paige, R., Pang, J., Patrangenaru, V., Ruymgaart, F., 2008. The one- and multi-sample problem for functional data with application to projective shape analysis. Journal of Multivariate Analysis (99), 815–833.

Nash, J., 1956. The embedding problem for Riemannian manifolds. Ann. of Math. 63, 20–63.

Palais, R. S., 1960. Slices and equivariant embeddings. In: Borel, A. (Ed.), Seminar on Transformation Groups. No. 46 in Annals of Mathematics Studies. Princeton Univ. Press, Princeton NJ, Ch. 8, pp. 101–115.

Schmidt, F. R., Clausen, M., Cremers, D., 2006. Shape matching by variational computation of geodesics on a manifold. In: Pattern Recognition (Proc. DAGM). Vol. 4174 of LNCS. Springer, Berlin, Germany, pp. 142–151.

Small, C. G., 1996. The Statistical Theory of Shape. Springer-Verlag, New York.

Zahn, C., Roskies, R., 1972. Fourier descriptors for plane closed curves. IEEE Trans. Computers C-21, 269–281.

Ziezold, H., 1977. Expected figures and a strong law of large numbers for random elements in quasi-metric spaces. Trans. 7th Prague Conf. Inf. Theory, Stat. Dec. Func., Random Processes A, 591–602.

Ziezold, H., 1994. Mean figures and mean shapes applied to biological figure and shape distributions in the plane. Biom. J. (36), 491–510.