Manifold stability and the central limit theorem for mean shape

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Abstract

In the literature there is an overwhelming number of concepts for a “mean” on shape spaces. First we classify those into three fundamental types. Then we introduce manifold stability which is essential to apply a standard two sample test on a non-manifold shape space. For sample means on Kendall’s shape spaces, we give the proof to establish manifold stability and illustrate consequences for the discrimination of non-concentrated shapes. We conclude with a discussion of the result for general shape spaces and population means.

1 Three Fundamental Types of Means

Suppose that a $X_1, \ldots, X_n \sim X$ are random elements on a Riemannian manifold $M$ which is embedded in a Euclidean space $\mathbb{R}^m$. Then the orthogonal projection $\Phi : \mathbb{R}^m \rightarrow M$ is well defined except possibly for a set of Lebesgue measure zero (Bhattacharya and Patrangenaru (2003)). If $d$ denotes the intrinsic distance on $M$ due to the Riemannian structure, $\| \cdot \|$ the Euclidean norm, $d\Phi$ the projection to the tangent space and $E$ the classical expectation we have the three fundamental types of possibly set-valued means:

<table>
<thead>
<tr>
<th>intrinsic</th>
<th>extrinsic</th>
<th>residual</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\arg\min_{p \in M} E(d(p, X)^2)$</td>
<td>$\arg\min_{p \in M} E(| p - X |^2)$</td>
<td>$\arg\min_{p \in M} E(| d\Phi_p(p - X) |^2)$</td>
</tr>
</tbody>
</table>

In particular, extrinsic means are as unique as the orthogonal projection is since they are equal to the set given by $\Phi(\mathbb{E}(X))$, (Hendriks and Landsman (1996); Bhattacharya and Patrangenaru (2003)). Moreover on spheres, residual means are identical to the set of dominating eigenvectors of $XX^T$, (Jupp (1988)).

In the modelling of shape, a compact Lie group $G$ (e.g. rotations) acts isometrically on $M$ giving the quotient shape space

$$\Sigma = M/G = \{ [p] : p \in M \}$$

$$[p] = \{ gp : g \in G \}$$

With $g_p \in \arg\min_{g \in G} \| p - gp \|$ define the following distances on the quotient

$$d^{(i)}_\Sigma([p], [p']) := \min_{g \in G} d(p, gp')$$

$$d^{(z)}_\Sigma([p], [p']) := \| p - g_p p' \|$$

$$d^{(z)}(p, [p]) := \| d\Phi p - g_p p' \|$$

to obtain the corresponding means on the quotient:

<table>
<thead>
<tr>
<th>intrinsic</th>
<th>Ziezold</th>
<th>Procrustean</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\arg\min_{[p] \in \Sigma} E(d^{(i)}_\Sigma([p], [X])^2)$</td>
<td>$\arg\min_{[p] \in \Sigma} E(d^{(z)}_\Sigma([p], [X])^2)$</td>
<td>$\arg\min_{[p] \in \Sigma} E(d^{(z)}([p], [X])^2)$</td>
</tr>
</tbody>
</table>

Most of the means in the literature are of one of these fundamental types, some of which are reported in Table 1. The so called partial Procrustes means on $\Sigma = SS^k_m$ are of all three types because in this case, all three of the above distances agree with one another.

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<table>
<thead>
<tr>
<th>concept in the literature</th>
<th>fundamental type</th>
</tr>
</thead>
<tbody>
<tr>
<td>center of gravity (Kobayashi and Nomizu (1969); Kendall (1977))</td>
<td>intrinsic</td>
</tr>
<tr>
<td>crude residuals (Jupp (1988))</td>
<td>residual</td>
</tr>
<tr>
<td>full Procrustes mean on ( \Sigma^k_m ) (Gower (1975))</td>
<td>Procrustean</td>
</tr>
<tr>
<td>mean figure (Ziezold (1994))</td>
<td>Ziezold</td>
</tr>
<tr>
<td>mean location (Hendriks and Landsman (1996))</td>
<td>extrinsic</td>
</tr>
<tr>
<td>partial Procrustes mean on ( S \Sigma^k_m ) (Dryden and Mardia (1998))</td>
<td>all</td>
</tr>
<tr>
<td>Schoenberg mean on ( R \Sigma^k_m ) (Bandulasiri et al (2009))</td>
<td>extrinsic</td>
</tr>
<tr>
<td>Veronese Whitney mean of ( \Sigma^2_k = \mathbb{C}P^{k-2} ) (Bhattacharya and Patrangenaru (2003))</td>
<td>extrinsic, Procrustean</td>
</tr>
</tbody>
</table>

Table 1: Classifying many concepts of means found in the literature.

2 Manifold Stability and the Central Limit Theorem

In general, a quotient space \( \Sigma = M/G \) of a Riemannian manifold modulo a compact Lie group \( G \) acting isometrically contains a dense manifold part \( \Sigma^* = M^*/G \), \( M^* \) is open and dense in \( M \) and a possibly non-void singular part \( \Sigma^0 = \Sigma \setminus \Sigma^* = M^0/G \), \( M^0 = M \setminus M^* \). With the isotropy group \( I_p = \{ g \in G : gp = p \} \) at \( p \in M \) we restrict ourselves to the case that \( I_p = \{ e \} \) for \( p \in M^* \) while \( I_p \neq \{ e \} \) for \( p = M^0 \).

If \( \mu_n \) is any of the above sample means and \( \mu \) a corresponding unique population mean then \( \mu_n \to \mu \) a.s. (Ziezold (1977); Bhattacharya and Patrangenaru (2003)) Further, if \( \mu \in \Sigma^* \) is unique, then under suitable conditions, there is a Central Limit Theorem

\[
\sqrt{n}(\phi(\mu_n) - \phi(\mu)) \overset{d}{\to} \mathcal{N}(0, \Sigma_\phi)
\]

with a covariance matrix \( \Sigma_\phi \) depending on a local chart \( \phi \) (Bhattacharya and Patrangenaru (2005); Hendriks and Landsman (1998); Huckemann (2010a)). Hence, 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. A similar two-sample test, however, requires the following property of manifold stability.

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

Example 2.1. Consider \( M = S^2 = \{(x, y, z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 = 1\} \) with the isometric action of \( S^1 = \{e^{i\phi} : \phi \in [0, \pi]\} \) given by \( e^{i\phi}(x, y, z) = (x \cos \phi, y \sin \phi, z) \). Then

\[
\Sigma = S^2/S^1 \cong [-1, 1] \cup \{-1\} \cup (-1, 1) \cup \{1\}.
\]

As depicted in Figure 1, suppose that the distribution of \( X \) on \( S^2 \) is uniform on \( \{(x, y, z) \in S^2 : 0 < x, y < 1, z = 0\} \) with total weight \( 1/3 \) combined with a point mass at the north pole \((0, 0, 1)\) of weight \( 2/3 \). Then the set of residual means is given by the north and south pole. Hence the set of Procrustean means of \([X]\) is precisely the singular part \( \Sigma^0 \).

In consequence we have the following.

Remark 2.2. In general Procrustean means are not manifold stable.

3 Manifold Stability for Samples on Kendall’s Shape Space

Recall that Kendall’s shape space \( \Sigma^k_m = S^k_m/\text{SO}(m) \) is the unit sphere \( S^k_m \) in the space of \( m \times (k-1) \) matrices modulo the special orthogonal group \( \text{SO}(m) \). Every \( m \times (k-1) \) matrix
Assume that contradiction unless that \( \mathbf{g} \) full Procrustes sample mean on Theorem 3.1. On \( \Sigma = \Sigma_m^k \), intrinsic and Ziezold sample means are manifold stable. A full Procrustes sample mean \( [p^*] \) of \( [X_1], \ldots, [X_n] \) is manifold stable if either \( m = 2 \) or if \( \langle p^*, g_{p^*} X_j \rangle \neq 0 \) for at least one \( j \in \{1, \ldots, n\} \) with any \( X_j \in [X_j] \in (\Sigma_m^k)^* \) and \( p^* \in [p^*] \).

**Proof.** Assume that \( p^* \in [p^*] \in \Sigma^0 \) while w.l.o.g \( X_1 \in \Sigma^* \). Moreover, w.l.o.g. we may assume that \( g_{p^*} X_j = X_j (j = 1, \ldots, n) \) as well as that there is \( e \neq g \in G \) such that \( 0 \neq d(p^*, gX_1) = d(p^*, X_1) \), i.e. \( \langle p^*, X_1 - gX_1 \rangle = 0 \), as well as \( gX_1 \neq X_1 \). Then using differentiation for the following first line and Lagrange minimization under constraining conditions for the latter two, obtain at once

\[
p^* \in \arg\min_{p \in \Sigma_m^k} \frac{1}{n} \sum_{j=1}^{n} d(X_j, p)^2 \quad \Rightarrow \quad \frac{1}{n} \sum_{j=1}^{n} (X_j - p^* \langle X_j, p^* \rangle) \frac{\arccos \langle p^*, X_j \rangle}{\|X_j - p^* \langle X_j, p^* \rangle\|} = 0 ,
\]

\[
p^* \in \arg\min_{p \in \Sigma_m^k} \frac{1}{n} \sum_{j=1}^{n} \|X_j - p\|^2 \quad \Rightarrow \quad \frac{1}{n} \sum_{j=1}^{n} (X_j - p^* \langle X_j, p^* \rangle) = 0 ,
\]

\[
p^* \in \arg\min_{p \in \Sigma_m^k} \frac{1}{n} \sum_{j=1}^{n} (1 - \langle X_j, p \rangle^2) \quad \Rightarrow \quad \frac{1}{n} \sum_{j=1}^{n} \langle X_j, p^* \rangle (X_j - p^* \langle X_j, p^* \rangle) = 0 .
\]

By hypothesis, in every line \( X_1 \) can be replaced by \( gX_1 \) without changing the value of the sums. In the first two lines, this yields the contradiction \( X_1 = gX_1 \). In the third line we only have this contradiction unless \( \langle p^*, X_1 \rangle = 0 \). This yields the assertion. \( \square \)

## 4 Discrimination Made Difficult for Full Procrustes Means

Here we consider on \( \Sigma = \Sigma_3^4 \) two maximally remote shapes \( \sigma_1 \) (1D) and \( \sigma_2 \) (2D) as depicted in Figure 2. Note that \( \sigma_1 \in \Sigma^0 \) while \( \sigma_2 \in \Sigma^* \). Below we report the percentages of successful discrimination of the following two groups.

- Group one consists six noisy versions of \( \sigma_1 \).
- Group two consists of one noisy version of \( \sigma_1 \) and five noisy versions of \( \sigma_2 \).

Multivariate normal isotropic noise with zero mean and standard deviation 0.01 has been added independently to every landmark. The discrimination has been based on a two-sample test of level 0.05 using tangent space coordinates obtained by orthogonal projection (for intrinsic and Ziezold means) and full Procrustes residuals (for full Procrustes means).

Figure 1: Left: uniform distribution on a quarter of the equator and a heavy point mass at the north pole (black) together with the two residual means at the poles (blue), unique extrinsic mean (red) and below the unique intrinsic mean (magenta). Right: distribution (black) and means projected to the quotient giving two Procrustean means (blue) and a unique Ziezold mean (red) and below a unique intrinsic mean (magenta).
Intrinsic means | Ziezold means | full Procrustes means
76 %          | 74 %        | 25 %

Table 2: Simulated power of a discrimination test of two groups using a two-sample test based on the respective means.

As shown in Table 2, the discrimination power of a two-sample test based on Procrustes means can be much smaller than that of intrinsic and Ziezold means, if the Procrustes mean is attained on or close to the non-manifold part $\Sigma^0$.

5 Discussion

With greater effort, namely introducing a horizontal lifting in optimal position on a twisted product (general shape spaces can be described by this extension of the concept of a fiber bundle), excluding only very artificial settings hardly occurring in practice, the result derived here for sample means can be extended to intrinsic and Ziezold population means on general shape spaces, thus fully justifying a two-sample test based on these means, (Huckemann (2010b)). Under slightly more restrictive side conditions, e.g. that a random shape has a non-vanishing density w.r.t. the projection of the spherical volume, manifold stability can also be established for full Procrustes means, (Huckemann (2011)).

Curiously, the general 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.

References


