

A Computable Characterization of the Extrinsic Mean of Reflection Shapes and Its Asymptotic Properties*

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Abstract

The reflection shapes of configurations in \mathbb{R}^m with k landmarks consist of all the geometric information that is invariant under compositions of similarity and reflection transformations. By considering the corresponding Schoenberg embedding, we embed the reflection shape space into the Euclidean space of all $(k-1)$ by $(k-1)$ real symmetric matrices. In this paper, we provide a computable formula of the extrinsic mean of the reflection shape in arbitrary dimensions. Moreover, the asymptotic analysis of the extrinsic mean of the reflection shapes is studied. By using the differentiability of spectral operators, we obtain a central limit theorem of the sample extrinsic mean of the reflection shapes. As a direct application, the two-example hypothesis test of the reflection shapes is also derived.

1 Introduction

The analysis of shape is one of the very early activities of human beings, which is of great interest in a wide variety of applications, such as morphometrics, biology, medical diagnosis, medical imaging, classification and many other fields. More applications of the shape analysis can be found from [10].

Shape is the geometrical information that remains when location, scale, rotation efforts are all removed from the object. Statistical shape analysis is based on the work of Kendall [16, 17] and Bookstein [7]. Following Kendall's definition [16], a shape space is the equivalent classes or the orbits of the configurations under the similarity transformation of translation, scaling and rotation. Since the shape spaces are usually no-Euclidean space, the standard statistical results on Euclidean spaces can not be applied directly. The basic concepts such as the *mean* of the random variables become non-trivial in statistical shape analysis. In fact, by embedding the shape space into certain metric space, the *Fréchet mean* can be defined as the minimizers of the generalized least squares problem, which is the generalization of the mean of the Euclidean space. However, depending on the different distances, there are many different means in statistical shape analysis. For instance, the famous *Procrustes mean* corresponds to the Procrustes distance (cf. [10, Chapter 5]); the Ziezold mean corresponds to the Ziezold distance (cf. [20]); the intrinsic and extrinsic means correspond to the intrinsic and extrinsic distances of the manifold, respectively (cf. e.g., [5]).

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In this paper, we mainly focus on the reflection shape space $\mathbb{R}\Sigma_m^k$ (see Section 2 for the definition). Moreover, as pointed out by [6, 3], it is simpler to carry out the extrinsic analysis on the reflection shape space both theoretically and computationally. The definition of the extrinsic mean on a non-Euclidean space was introduced independently by Hendricks and Landsman [15] and Patrangenaru [18]. For the reflection shape space, Dryden et al. [11] and Bhattacharya [3] presented two computable formulas of the extrinsic mean shape. However, both may not be the *true* extrinsic mean shape formula since both used formulas that are not the true formulas of the projections. Actually, it is well-known that the reflection shape space can be embedded into the $(k-1)$ by $(k-1)$ real symmetric matrices space \mathcal{S}^{k-1} by the Schoenberg mapping J (see (2) for the definition). It follows from [5, Proposition 3.1] that in order to compute the extrinsic means of the reflection shapes, we must first study the characterization of the projections over the closed subset $J(\mathbb{R}\Sigma_m^k)$ defined in the Euclidean space \mathcal{S}^{k-1} , which is provided in Proposition 2 in Section 3. As the consequence, we deduce the correct extrinsic mean reflection shape formula, which further implies that the resulting extrinsic sample mean shape is a strongly consistent estimator (cf. [5, Theorem 2.3]).

In the second part of this paper, we conduct an asymptotic analysis of the sample extrinsic mean reflection shape. More precisely, as the direct application of the differentiability of spectral operators (see [8, 9]) and the classical convergence result in probability [1] (see Lemma 1), we derive the asymptotic distribution of the sample extrinsic mean reflection shape. It is worth to point out that for the general extrinsic mean on manifold, the corresponding asymptotic distribution of the sample extrinsic mean can be obtained from [6]. By the central limit theorem obtained in this paper, we are able to apply many standard statistical results to the reflection shape space. For example, we develop the generalized Hotelling T^2 test to distinguish two distributions of reflection shapes by comparing their sample extrinsic means in this paper. It also can be seen from the numerical simulation that the test based on the obtained extrinsic sample mean of the reflection space performs quite well with respect to the other means such as the Procrustes mean, the Ziezold mean and intrinsic means, which are usually time-consuming for applications of a large sample size.

The remaining parts of this paper are organized as follows. In Section 2, we briefly introduce some basic concepts in shape analysis. We define and present the explicit formula of the extrinsic mean of the reflection shapes in Section 3. The asymptotic analysis of the sample extrinsic mean of the reflection shapes is conducted in Section 4. Finally, we present the generalized Hotelling T^2 test for the reflection shapes and report the numerical results in the last section.

Notation. Let $\mathbb{R}^{m \times n}$ be the Euclidean space of $m \times n$ real matrices with the trace inner product $\langle X, Y \rangle := \text{trace}(X^T Y)$ for $X, Y \in \mathbb{R}^{m \times n}$ and its induced norm $\|\cdot\|$. Let $\mathcal{S}^m \subseteq \mathbb{R}^{m \times m}$ be the Euclidean space of $m \times m$ real symmetric matrices. Let \mathcal{S}_+^m be the closed convex cone of all $m \times m$ positive semidefinite matrices. We use \mathcal{O}^p to denote the set of $p \times p$ orthogonal matrices.

- For any $X \in \mathbb{R}^{m \times n}$, denote X_{ij} the (i, j) -th entry of X .
- For any $X \in \mathbb{R}^{m \times n}$ and a given index set $\mathcal{J} \subseteq \{1, \dots, n\}$, we use $X_{\mathcal{J}}$ to denote the sub-matrix of X obtained by removing all the columns of X not in \mathcal{J} . In particular, we use x_j to represent the j -th column of X , $j = 1, \dots, n$.
- Let $\mathcal{I} \subseteq \{1, \dots, m\}$ and $\mathcal{J} \subseteq \{1, \dots, n\}$ be two index sets. For any $X \in \mathbb{R}^{m \times n}$, we use $X_{\mathcal{I}\mathcal{J}}$ to denote the $|\mathcal{I}| \times |\mathcal{J}|$ sub-matrix of X obtained by removing all the rows of X not in \mathcal{I} and all the columns of X not in \mathcal{J} .
- We use “ \circ ” to denote the Hardamard product between matrices, i.e., for any two matrices A and B in $\mathbb{R}^{m \times n}$ the (i, j) -th entry of $X := A \circ B \in \mathbb{R}^{m \times n}$ is $X_{ij} = A_{ij} B_{ij}$.

- Let $\text{diag}(\cdot) : \mathbb{R}^m \rightarrow \mathcal{S}^m$ be a linear mapping defined by for any $x \in \mathbb{R}^m$, $\text{diag}(x)$ denotes the diagonal matrix whose i -th diagonal entry is x_i , $i = 1, \dots, m$.

2 The reflection shape space

We start from introducing some basic concepts in shape analysis and we mainly focus on the reflection shape, which is briefly introduced below.

Given an object, we are interested in the geometrical information that remains when location, scale, rotational and reflection efforts are all removed out from the object. Following the definition introduced by Kendall [16], this geometrical information is so-called the *reflection shape* of an object. Therefore, it is clear that the reflection shape of an object is invariant under the similarity transformations of translation, scaling, rotation and reflection.

In applications, a finite number of points are located on each object based on some prior decided criterions. We call these points the *landmarks* of the object. Each object in \mathbb{R}^m can be represented by the corresponding k landmarks. Without loss of generality, for each object, we always assume that $k > m$ and not all landmarks being the same. Usually, the configuration of k landmarks is called k -ad. In statistical shape analysis, the configuration in \mathbb{R}^m with k landmarks or the k -ad is represented by an $m \times k$ matrix X , whose j -th column is the coordinates of the j -th landmark under some chosen coordinate system, i.e.,

$$X = [x_1, \dots, x_k] \in \mathbb{R}^{m \times k},$$

where $x_j \in \mathbb{R}^m$, $j = 1, \dots, k$ are the landmark coordinate vectors.

The reflection shape of a k -ad $X \in \mathbb{R}^{m \times k}$ is the equivalence class or the orbit under the similarity transformations of translation, scaling, rotation and reflection. First, we remove the effect of translation by using the standard Helmert sub-matrix (cf. [10, Definition 2.5]). For the given positive integer k , the corresponding Helmert sub-matrix $H^k \in \mathbb{R}^{k \times (k-1)}$ (cf. [10, Definition 2.5]) is given by

$$H^k = [h_1^k, \dots, h_{k-1}^k] \in \mathbb{R}^{k \times (k-1)},$$

where for each $j \in \{1, \dots, k-1\}$, the column vector $h_j^k \in \mathbb{R}^k$ consists of $-1/\sqrt{j(j+1)}$ repeated j times, followed by $j/\sqrt{j(j+1)}$ and then $k-j-1$ zeros, i.e.,

$$h_j^k = \left(-1/\sqrt{j(j+1)}, \dots, -1/\sqrt{j(j+1)}, j/\sqrt{j(j+1)}, 0, \dots, 0 \right)^T \in \mathbb{R}^k.$$

We note that each column is orthogonal to the vector of e of all ones in \mathbb{R}^k and

$$H^k (H^k)^T = I_k - \frac{1}{k} e e^T \quad \text{and} \quad (H^k)^T H_k = I_{k-1},$$

where I_k is the identity matrix of size k . Therefore, the given k -ad X can be centered by right multiplying H^k , i.e.,

$$Z = X H^k \in \mathbb{R}^{m \times (k-1)}.$$

To remove the effect of scaling, we consider the normalized centered k -ad $\mathfrak{X} \in \mathbb{R}^{m \times (k-1)}$ of X , i.e.,

$$\mathfrak{X} = \frac{Z}{\|Z\|}, \quad Z = X H^k, \tag{1}$$

which is called the *preshape* of the k -ad X . It is clear that the preshape of any given k -ad lies on the unit sphere of $\mathbb{R}^{m \times (k-1)}$. We call the unit sphere of $\mathbb{R}^{m \times (k-1)}$ the *preshape sphere* and denoted by

$$\mathfrak{S}_m^k := \left\{ \mathfrak{X} \in \mathbb{R}^{m \times (k-1)} \mid \|\mathfrak{X}\| = 1 \right\}.$$

Finally, the reflection shape of the k -ad X is the orbit (equivalent class) of the preshape $\mathfrak{X} \in \mathfrak{S}_m^k$ of X under left multiplication by the $m \times m$ orthogonal matrix, i.e.,

$$[\mathfrak{X}]_{RS} := \{R\mathfrak{X} \mid R \in \mathcal{O}^m\}.$$

Therefore, the reflection shape space is defined as

$$\text{R}\Sigma_m^k := \left\{ [\mathfrak{X}]_{RS} \mid \mathfrak{X} \in \mathfrak{S}_m^k \right\}.$$

Let \mathcal{S}^{k-1} denote the space of all $k-1$ by $k-1$ real symmetric matrices. The Schoenberg mapping $J : \text{R}\Sigma_m^k \rightarrow \mathcal{S}^{k-1}$ is given by

$$J([\mathfrak{X}]_{RS}) = \mathfrak{X}^T \mathfrak{X}, \quad (2)$$

where $\mathfrak{X} \in \mathfrak{S}_m^k$ is the preshape of a k -ad X given by (1). Define $J(\text{R}\Sigma_m^k)$ to be the range of J , i.e.,

$$J(\text{R}\Sigma_m^k) = \mathcal{S}_+^{k-1}(m) := \left\{ Y \in \mathcal{S}^{k-1} \mid Y \in \mathcal{S}_+^{k-1}, \text{trace}(Y) = 1, 1 \leq \text{rank}(Y) \leq m \right\}.$$

We know from [11] that the Schoenberg mapping is a homeomorphism from the reflection shape space to $\mathcal{S}_+^{k-1}(m)$. Moreover, it is well-known that (see e.g., [3, 4]) that the Schoenberg mapping J is an embedding of the reflection shape space $\text{R}\Sigma_m^k$. We would like to point out that among the possible embedding of the reflection shape space, the Schoenberg mapping is an *equivalent embedding* which preserves many geometric features of $\text{R}\Sigma_m^k$ (see [5, 6] for more details).

The range $\mathcal{S}_+^{k-1}(m)$ of the reflection shape space under J is a closed subset of the Euclidean space \mathcal{S}^{k-1} with the norm $\|\cdot\|$. Therefore, the embedding J also induces a metric of the reflection shape space $\text{R}\Sigma_m^k$, i.e.,

$$\rho^e([\mathfrak{X}]_{RS}, [\mathfrak{X}']_{RS}) = \|J([\mathfrak{X}]_{RS}) - J([\mathfrak{X}']_{RS})\|. \quad (3)$$

We call the metric ρ^e the *extrinsic distance* of $\text{R}\Sigma_m^k$. Therefore, the reflection shape space can be considered as a metric space $(\text{R}\Sigma_m^k, \rho^e)$.

3 Extrinsic mean of reflection shapes

Since the reflection shape space $\text{R}\Sigma_m^k$ is a metric space with the metric ρ^e defined in (3), the extrinsic mean of reflection shapes can be defined as the Fréchet mean under the extrinsic distance. We give the details below.

Let (\mathcal{M}, ρ) be a metric space where ρ is a metric on \mathcal{M} . Denote \mathcal{B} the Borel σ -algebra of (\mathcal{M}, ρ) . Recall that a \mathcal{M} -valued random variable X is a measurable function from an abstract probability space $(\Omega, \mathcal{A}, \mathbb{P})$ into $(\mathcal{M}, \mathcal{B})$, where “*measurable*” refers to the corresponding Borel σ -algebra \mathcal{B} .

Let \mathcal{Q} be a given *probability measure* of \mathcal{M} , i.e., the probability distribution of a given \mathcal{M} -valued random variable X . The corresponding Fréchet function is defined as

$$F_{\mathcal{Q}}(x) = \int_{\mathcal{M}} \rho^2(\omega, x) \mathcal{Q}(d\omega), \quad x \in \mathcal{M}. \quad (4)$$

Then, the general mean of \mathcal{Q} on the metric space introduced by Fréchet [12] can be defined as the minimizers of the Fréchet function $F_{\mathcal{Q}}$. More precisely, if there exists some $x \in \mathcal{M}$ such that the Fréchet function value $F_{\mathcal{Q}}(x) < \infty$, then we call the set of minimizers of $F_{\mathcal{Q}}$ on \mathcal{M} the *Fréchet mean set* of \mathcal{Q} . Moreover, if the Fréchet mean set of the given probability measure \mathcal{Q} is a singleton, then we say the *Fréchet mean* of \mathcal{Q} exists and denote it by $\mu_{\mathcal{Q}}$.

Let X_1, \dots, X_n be independently and identically distributed (i.i.d.) \mathcal{M} -valued random variables with the common distribution \mathcal{Q} . Consider their empirical distribution $\mathcal{Q}_n := \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$, where δ_{X_i} are the Dirac measure of X_i , $i = 1, \dots, n$. Then, the Fréchet mean set of \mathcal{Q}_n is called the *sample Fréchet mean set* of \mathcal{Q} , if there exists some $x \in \mathcal{M}$ such that

$$F_{\mathcal{Q}_n}(x) = \frac{1}{n} \sum_{i=1}^n \rho^2(X_i, x) < \infty.$$

Also, if the sample Fréchet mean set of \mathcal{Q} is a singleton, then we say that the *sample Fréchet mean* of \mathcal{Q} exists and denote it by $\bar{\mu}_{\mathcal{Q}}$.

In particular, for the given probability measure \mathcal{Q} in the reflection shape space $(\mathbf{R}\Sigma_m^k, \rho^e)$, we call the corresponding Fréchet mean (set) the *extrinsic mean (set)* and the sample Fréchet mean (set) the *sample extrinsic mean (set)*, respectively. Since $\mathcal{S}_+^{k-1}(m)$ is a compact subspace, we know from [5, Theorem 2.1] that the extrinsic mean set and the sample extrinsic mean set of the given probability measure \mathcal{Q} on $(\mathbf{R}\Sigma_m^k, \rho^e)$ are nonempty and compact. Moreover, if the probability measure \mathcal{Q} has a unique extrinsic mean, then it follows from [5, Theorem 2.3] that any measurable selection from the sample Fréchet mean set is a strongly consistent estimator of $\mu_{\mathcal{Q}}$.

Since the range $\mathcal{S}_+^{k-1}(m)$ is a closed subset in \mathcal{S}^{k-1} , for every given $Z \in \mathcal{S}^{k-1}$ there exists a compact set in $\mathcal{S}_+^{k-1}(m)$ whose distance from Z is the smallest among all points in $\mathcal{S}_+^{k-1}(m)$. We call this set the projections of $Z \in \mathcal{S}^{k-1}$ on $\mathcal{S}_+^{k-1}(m)$ and denote it by

$$\Pi_{\mathcal{S}_+^{k-1}(m)}(Z) := \left\{ Z^* \in \mathcal{S}_+^{k-1}(m) \mid \|Z^* - Z\| \leq \|Y - Z\| \ \forall Y \in \mathcal{S}_+^{k-1}(m) \right\}.$$

Therefore, since the reflection shape space is embedded into the Euclidean space \mathcal{S}^{k-1} by the Schoenberg embedding, we can obtain the characterization of the extrinsic (sample) means by considering the corresponding projections of the mean of random variables in \mathcal{S}^{k-1} . The following proposition is taken from [5, Proposition 3.1].

Proposition 1 *Let \mathcal{Q} be a given probability measure of the reflection shape space $(\mathbf{R}\Sigma_m^k, \rho^e)$. Let J be the Schoenberg embedding defined in (2). Denote $\tilde{\mathcal{Q}} := \mathcal{Q} \circ J^{-1}$ the image of \mathcal{Q} , which is a probability measure in \mathcal{S}^{k-1} . Then, the extrinsic mean set of \mathcal{Q} is given by $J^{-1}(\Pi_{\mathcal{S}_+^{k-1}(m)}(\mu_{\tilde{\mathcal{Q}}}))$, where $\mu_{\tilde{\mathcal{Q}}}$ is the classical expected value (mean) of $\tilde{\mathcal{Q}}$ in the Euclidean space \mathcal{S}^{k-1} , i.e.,*

$$\mu_{\tilde{\mathcal{Q}}} = \int_{\mathcal{S}^{k-1}} Y \tilde{\mathcal{Q}}(dY).$$

Next, we shall study the formula of the projections $\Pi_{\mathcal{S}_+^{k-1}(m)}(Z)$ for a given $Z \in \mathcal{S}^{k-1}$, which is the solution set of the following nonconvex optimization problem

$$\begin{aligned} \min \quad & \frac{1}{2} \|Y - Z\|^2 \\ \text{s.t.} \quad & \text{trace}(Y) = 1, \quad \text{rank}(Y) \leq m, \\ & Y \in \mathcal{S}_+^{k-1}. \end{aligned}$$

For the given $Z \in \mathcal{S}^{k-1}$, denote $\lambda(Z) = (\lambda_1(Z), \lambda_2(Z), \dots, \lambda_{k-1}(Z))^T$ with the eigenvalues $\lambda_1(Z) \geq \lambda_2(Z) \geq \dots \geq \lambda_{k-1}(Z)$ of Z arranging in the non-increasing order. Let $\nu_1(Z) > \dots > \nu_r(Z)$ be the distinct eigenvalues of Z . For each $s \in \{1, \dots, r\}$, define the index set

$$a_s = \{j \in \{1, \dots, k-1\} \mid \lambda_j(Z) = \nu_s(Z)\}. \quad (5)$$

Let $Z = P\Lambda(Z)P^T$ be the eigenvalue decomposition of Z , where $\Lambda(Z) = \text{diag}(\lambda(Z))$ is the diagonal matrix whose i -th diagonal item is $\lambda_i(Z)$, $i = 1, \dots, k-1$ and $P \in \mathcal{O}^{k-1}$ is the $(k-1) \times (k-1)$ orthogonal matrix. For the given $Z \in \mathcal{S}^{k-1}$, define

$$\theta_j(Z) := \frac{\sum_{i=1}^j \lambda_i(Z) - 1}{j}, \quad j = 1, \dots, m. \quad (6)$$

Let $\kappa \in \{1, \dots, m\}$ be the largest index such that $\lambda_\kappa(Z) > \theta_\kappa(Z)$, i.e.,

$$\kappa := \max \{j \in \{1, \dots, m\} \mid \lambda_j(Z) > \theta_j(Z)\}. \quad (7)$$

Moreover, define the index sets α , β , and γ respectively by

$$\alpha := \{j \in \{1, \dots, k-1\} \mid \lambda_j(Z) > \lambda_m(Z)\} \quad (8)$$

$$\beta := \{j \in \{1, \dots, k-1\} \mid \lambda_j(Z) = \lambda_m(Z)\} \quad (9)$$

$$\gamma := \{j \in \{1, \dots, k-1\} \mid \lambda_j(Z) < \lambda_m(Z)\} \quad (10)$$

For the given $Z \in \mathcal{S}^{k-1}$, let $g : \mathbb{R}^{k-1} \rightarrow \mathbb{R}^{k-1}$ be a vector-valued function defined on the eigenvalue vector of $\lambda(Z)$ by

$$g(\lambda(Z)) = (g_1(\lambda(Z)), \dots, g_{k-1}(\lambda(Z)))^T \in \mathbb{R}^{k-1}$$

with

$$g_j(\lambda(Z)) = \begin{cases} \lambda_j(Z) - \theta_\kappa(Z) & \text{if } 1 \leq j \leq \kappa, \\ 0 & \text{otherwise,} \end{cases} \quad j = 1, \dots, k-1. \quad (11)$$

Thus, the projections $\Pi_{\mathcal{S}_+^{k-1}(m)}(Z)$ for the given $Z \in \mathcal{S}^{k-1}$ can be characterized as follows.

Proposition 2 *Let $Z = P\Lambda(Z)P^T$ be the eigenvalue decomposition of Z . Then,*

$$\Pi_{\mathcal{S}_+^{k-1}(m)}(Z) = \left\{ [P_\alpha \ P_\beta Q \ P_\gamma] \text{diag}(g(\lambda(Z))) [P_\alpha \ P_\beta Q \ P_\gamma]^T \mid Q \in \mathcal{O}^{|\beta|} \right\}. \quad (12)$$

Proof. It follows from Ky Fan's inequality (cf. [2, (IV.62)]), we know that $Z^* \in \Pi_{\mathcal{S}_+^{k-1}(m)}(Z)$ if and only if Z and Z^* have a simultaneous ordered eigenvalue decomposition (i.e., there exists $U \in \mathcal{O}^{k-1}$ such that $Z = U\Lambda(Z)U^T$ and $Z^* = U\Lambda(Z^*)U^T$), and the eigenvalues of Z^* is the optimal solution of the following simple optimization problem

$$\begin{aligned} \min \quad & \frac{1}{2} \|y - \lambda(Z)\|^2 \\ \text{s.t.} \quad & \sum_{i=1}^{k-1} y_i = 1, \\ & y_1 \geq y_2 \geq \dots \geq y_m \geq y_{m+1} = \dots = y_{k-1} = 0. \end{aligned}$$

It follows from the classical KKT condition that $g(\lambda(Z))$ defined in (11) is the unique optimal solution of this convex problem. Furthermore, since

$$P^T U \Lambda(Z) U^T P = \Lambda(Z),$$

it can be checked directly that $P^T U \in \mathcal{O}^{k-1}$ has the block diagonal structure, i.e.,

$$P^T U = \text{diag}((P^T U)_{a_1 a_1}, \dots, (P^T U)_{a_r a_r}) \quad \text{with} \quad (P^T U)_{a_s a_s} \in \mathcal{O}^{|a_s|}, \quad s = 1, \dots, r.$$

Therefore, from the definition of $g(\lambda(Z))$, we know that $Z^* \in \Pi_{\mathcal{S}_+^{k-1}(m)}(Z)$ if and only if there exists $Q \in \mathcal{O}^{|\beta|}$ such that

$$Z^* = [P_\alpha \ P_\beta Q \ P_\gamma] \text{diag}(g(\lambda(Z))) [P_\alpha \ P_\beta Q \ P_\gamma]^T.$$

This completes the proof. \square

For the given Z , define the subset β_1 and β_2 of the index set β by

$$\beta_1 := \{j \in \{1, \dots, m\} \mid \lambda_j(Z) = \lambda_m(Z)\} \quad \text{and} \quad \beta_2 := \{j \in \{m+1, \dots, k-1\} \mid \lambda_j(Z) = \lambda_m(Z)\}.$$

From (12), we know that the projection set $\Pi_{\mathcal{S}_+^{k-1}(m)}(Z)$ is singleton if and only if $\kappa \notin \beta_1$ or $\beta_2 = \emptyset$ for the given Z . Therefore, by combining with Proposition 1, we have the following corollary on the extrinsic mean of the reflection shape.

Corollary 1 *Let \mathcal{Q} be a given probability measure on the reflection shape space $(\mathbb{R}\Sigma_m^k, \rho^e)$. Then, the extrinsic mean of \mathcal{Q} exists if and only if the expect value $\mu_{\tilde{\mathcal{Q}}}$ of the probability distribution $\tilde{\mathcal{Q}} = \mathcal{Q} \circ J^{-1}$ in \mathcal{S}^{k-1} satisfies that*

$$\kappa \notin \beta_1 \quad \text{or} \quad \lambda_m(\mu_{\tilde{\mathcal{Q}}}) > \lambda_{m+1}(\mu_{\tilde{\mathcal{Q}}}), \quad (13)$$

where κ and $\theta_m(\mu_{\tilde{\mathcal{Q}}})$ are defined with respect to the symmetric matrix $\mu_{\tilde{\mathcal{Q}}}$ by (7) and (6), respectively.

For the given $Z \in \mathcal{S}^{k-1}$, if the index set $\beta = \beta_1 \cup \beta_2$ is empty, then we know that the projection $\Pi_{\mathcal{S}_+^{k-1}(m)}$ is a matrix-valued function which is well-defined on a neighborhood of $Z \in \mathcal{S}^{k-1}$ (also known as the spectral operator according to [8, 9]). Moreover, we know from [8, Theorem 3.6 & 3.11] that the $\Pi_{\mathcal{S}_+^{k-1}(m)}$ is also twice continuously differentiable at Z , i.e., for any $\mathcal{S}^{k-1} \ni H \rightarrow 0$,

$$\Pi_{\mathcal{S}_+^{k-1}(m)}(Z + H) - \Pi_{\mathcal{S}_+^{k-1}(m)}(Z) = \Pi'_{\mathcal{S}_+^{k-1}(m)}(Z)H + O(\|H\|^2), \quad (14)$$

where $\Pi'_{\mathcal{S}_+^{k-1}(m)}(Z)$ at Z is the derivative of $\Pi_{\mathcal{S}_+^{k-1}(m)}$ at Z given by

$$\Pi'_{\mathcal{S}_+^{k-1}(m)}(Z)H = P (\Xi \circ P^T H P) P^T - P \begin{bmatrix} \frac{1}{\kappa} \text{tr}(P_\alpha^T H P_\alpha) I_{|\alpha|} & 0 \\ 0 & 0 \end{bmatrix} P^T, \quad (15)$$

where the symmetric matrix $\Xi \in \mathcal{S}^{k-1}$ is defined by

$$\Xi_{ij} := \begin{cases} 1 & \text{if } 1 \leq i, j \leq \kappa, \\ \frac{\lambda_i(Z) - \theta_\kappa(Z)}{\lambda_i(Z) - \lambda_j(Z)} & \text{if } 1 \leq i \leq \kappa \text{ and } \kappa + 1 \leq j \leq k-1, \\ \frac{-\lambda_j(Z) + \theta_\kappa(Z)}{\lambda_i(Z) - \lambda_j(Z)} & \text{if } \kappa + 1 \leq i \leq k-1 \text{ and } 1 \leq j \leq \kappa, \\ 0 & \text{otherwise,} \end{cases} \quad i, j = 1, \dots, k-1.$$

4 The asymptotic analysis of the extrinsic mean

In this section, we always assume that the extrinsic mean $\mu_{\mathcal{Q}}$ of probability measure \mathcal{Q} on the reflection shape space $(\mathbf{R}\Sigma_m^k, \rho^e)$ exists, which implies that the mean $\mu_{\tilde{\mathcal{Q}}}$ of the probability distribution $\tilde{\mathcal{Q}} = \mathcal{Q} \circ J^{-1}$ in \mathcal{S}^{k-1} satisfies condition (13) and the projection $\Pi_{\mathcal{S}_+^{k-1}(m)}$ is well-defined in a neighborhood of $\mu_{\tilde{\mathcal{Q}}}$ in \mathcal{S}^{k-1} and differentiable at $\mu_{\tilde{\mathcal{Q}}}$ with the derivative $\Pi'_{\mathcal{S}_+^{k-1}(m)}$ given by (15).

Let X_1, X_2, \dots be a sequence of i.i.d. random variables in the reflection shape space $(\mathbf{R}\Sigma_m^k, \rho^e)$ with the common probability measure \mathcal{Q} . Since the Schoenberg mapping J given by (2) is a homeomorphism, we know that the images $Y_1 = J(X_1), Y_2 = J(X_2), \dots$ is a sequence of i.i.d. random variables in the Euclidean space \mathcal{S}^{k-1} with the common probability measure $\tilde{\mathcal{Q}} = \mathcal{Q} \circ J^{-1}$. For the given sample size n , let $\bar{Y}_n = \frac{1}{n} \sum_{i=1}^n Y_i$ be the sample mean. Then, we

know from the strong law of large numbers that \bar{Y}_n converges to the mean $\mu_{\tilde{\mathcal{Q}}}$ almost surely as $n \rightarrow \infty$. Therefore, we know that for a sufficiently large sample size n , the projection mapping $\Pi_{\mathcal{S}_+^{k-1}(m)}$ is well-defined at the sample mean \bar{Y}_n almost surely.

Let us further assume that the common distribution of the i.i.d. random variables Y_1, \dots, Y_n in \mathcal{S}^{k-1} has the covariance matrix Σ (under certain orthogonal base of \mathcal{S}^{k-1}). It follows from the multivariate central limit theorem that the distribution of $G_n := \sqrt{n}(\bar{Y}_n - \mu_{\tilde{\mathcal{Q}}})$ converges to a Gaussian distribution with zero mean and the covariance Σ as $n \rightarrow \infty$, i.e.,

$$G_n = \sqrt{n}(\bar{Y}_n - \mu_{\tilde{\mathcal{Q}}}) \xrightarrow{d} G,$$

where G is a symmetric random matrix with this limit Gaussian distribution. The following lemma is taken from Anderson [1], which is important for our analysis.

Lemma 1 *Let \mathcal{E} and \mathcal{E}' be two given Euclidean space. Let U_n be a given \mathcal{E} -valued random variable defined on a probability space $(\Omega, \mathcal{A}, \mathbb{P})$. Suppose that U_n converges in distribution to the \mathcal{E} -valued random variable U . For each n , let $F_n : \mathcal{E} \rightarrow \mathcal{E}'$ be a given function, and let V_n be the \mathcal{E}' -valued random variable defined by $V_n = F_n(U_n)$. Assume that there exists a function $F : \mathcal{E} \rightarrow \mathcal{E}'$ such that for every continuity point Y of F ,*

$$\lim_{n \rightarrow \infty} F_n(Y_n) = F(Y) \quad \text{as} \quad \lim_{n \rightarrow \infty} Y_n = Y.$$

If the probability of the set of discontinuities of F in \mathcal{E} is zero, then we have

$$V_n \xrightarrow{d} V \quad \text{as} \quad n \rightarrow \infty,$$

where V is the \mathcal{E}' -valued random variable given by $V = F(U)$.

The following results are on the asymptotic distribution of the extrinsic mean of the reflection shapes.

Theorem 1 *Let X_1, \dots, X_n be a sequence of i.i.d. random variables in the reflection shape space $(\mathbf{R}\Sigma_m^k, \rho^e)$ with the common probability measure \mathcal{Q} . Assume that the extrinsic mean of \mathcal{Q} exists. Let $\bar{Y}_n = \frac{1}{n} \sum_{i=1}^n Y_i$ be the sample mean of $Y_i = J(X_i)$, $i = 1, \dots, n$, and let $\mu_{\tilde{\mathcal{Q}}}$ be*

the mean of the image probability distribution $\tilde{\mathcal{Q}}$. Let G be the random matrix with the limit distribution of $G_n = \sqrt{n}(\bar{Y}_n - \mu_{\tilde{\mathcal{Q}}})$. Then, we have

$$\sqrt{n} \left(\Pi_{\mathcal{S}_+^{k-1}(m)}(\bar{Y}_n) - \Pi_{\mathcal{S}_+^{k-1}(m)}(\mu_{\tilde{\mathcal{Q}}}) \right) \xrightarrow{d} Z \quad \text{as } n \rightarrow \infty,$$

where Z is a symmetric random matrix given by $\Pi'_{\mathcal{S}_+^{k-1}(m)}(\mu_{\tilde{\mathcal{Q}}})(G)$.

Proof. Since the extrinsic mean of \mathcal{Q} exists, we know that the projection $\Pi_{\mathcal{S}_+^{k-1}(m)}$ is continuously differentiable in a neighborhood of $\mu_{\tilde{\mathcal{Q}}}$. It is clear that the derivative function $F := \Pi'_{\mathcal{S}_+^{k-1}(m)}(\mu_{\tilde{\mathcal{Q}}})$ is continuous everywhere over \mathcal{S}^{k-1} . Suppose that $H \in \mathcal{S}^{k-1}$ is arbitrarily chosen. Let $H_n \in \mathcal{S}^{k-1}$ be a sequence converging to H . For the sufficiently large n , we define

$$F_n(H_n) := \sqrt{n} \left(\Pi_{\mathcal{S}_+^{k-1}(m)}(\mu_{\tilde{\mathcal{Q}}} + \frac{H_n}{\sqrt{n}}) - \Pi_{\mathcal{S}_+^{k-1}(m)}(\mu_{\tilde{\mathcal{Q}}}) \right).$$

Therefore, we know from (14) that

$$\lim_{n \rightarrow \infty} F_n(H_n) = F(H).$$

Thus, the desired result follows directly from Lemma 1. \square

It is well-known that the eigenvalues and eigenvectors of symmetric matrices have the following perturbation properties: for any given $Z \in \mathcal{S}^{k-1}$ with eigenvalue decomposition $Z = P(Z)\Lambda(Z)P(Z)^T$ and any $\mathcal{S}^{k-1} \ni H \rightarrow 0$,

$$\Lambda_{a_s a_s}(Z + H) - \Lambda_{a_s a_s}(Z) = \Lambda(P_{a_s}(Z)^T H P_{a_s}(Z)) + O(\|H\|^2), \quad s = 1, \dots, r,$$

where a_s , $s = 1, \dots, r$ are defined by (5) with respect to Z . Moreover, for the given $Z \in \mathcal{S}^{k-1}$, if we define the functions $\mathcal{P}_s : \mathcal{S}^{k-1} \rightarrow \mathcal{S}^{k-1}$, $s = 1, \dots, r$ by

$$\mathcal{P}_s(Y) = \sum_{i \in a_s} P_i(Y) P_i(Y)^T \quad \text{for any } Y = P(Y)\Lambda(Y)P(Y)^T,$$

then \mathcal{P}_s , $s = 1, \dots, r$ are twice continuously differentiable near Z , which implies that for any $\mathcal{S}^{k-1} \ni H \rightarrow 0$,

$$\mathcal{P}_s(Z + H) - \mathcal{P}_s(Z) = \mathcal{P}'_s(Z)H + O(\|H\|^2), \quad s = 1, \dots, r,$$

where the derivative $\mathcal{P}'_s(Z)$, $s = 1, \dots, r$ are given by

$$\mathcal{P}'_s(Z)H = P(Z)^T [\Omega_s(Z) \circ P(Z)^T H P(Z)] P(Z)^T$$

with

$$(\Omega_s(Z))_{ij} = \begin{cases} \frac{1}{\lambda_i(Z) - \lambda_j(Z)} & \text{if } i \in a_s, j \in a_{s'}, s' \neq s, \\ -1 & \text{if } i \in a_{s'}, j \in a_s, s' \neq s, \\ 0 & \text{otherwise,} \end{cases} \quad i, j = 1, \dots, k-1.$$

Let Y_1, \dots, Y_n in \mathcal{S}^{k-1} be a sequence of the i.i.d. random matrices with the mean μ and \bar{Y}_n be the corresponding sample mean. Let G be the random matrix with the limit distribution of $\sqrt{n}(\bar{Y}_n - \mu)$. Then, by the similar argument of Theorem 1, we obtain from Lemma 1 that as $n \rightarrow \infty$

$$\sqrt{n} (\Lambda_{a_s a_s}(\bar{Y}_n) - \Lambda_{a_s a_s}(\mu)) \xrightarrow{d} \Lambda(P_{a_s}(\mu)^T G P_{a_s}(\mu)), \quad s = 1, \dots, r$$

and

$$\sqrt{n} (\mathcal{P}_s(\bar{Y}_n) - \mathcal{P}_s(\mu)) \xrightarrow{d} \mathcal{P}'_s(\mu)G, \quad s = 1, \dots, r,$$

where all index sets a_s are defined with respect to the mean μ .

5 Two-sample test on the reflection shape space

As an application of the obtained asymptotic distribution of the sample extrinsic mean, we can construct the statistical test to compare two probability distributions \mathcal{Q}_1 and \mathcal{Q}_2 on the reflection shape space $(\mathbb{R}\Sigma_m^k, \rho^e)$.

Let X_1^1, \dots, X_n^1 and X_1^2, \dots, X_n^2 be two i.i.d. samples from \mathcal{Q}_1 and \mathcal{Q}_2 respectively. For simplicity, we also assume that they are mutually independent. Suppose that the extrinsic means of \mathcal{Q}_1 and \mathcal{Q}_2 exist, denoted by $\mu_{\mathcal{Q}_1}$ and $\mu_{\mathcal{Q}_2}$, respectively. The hypothesis which we want to test is

$$H_0 : \mathcal{Q}_1 = \mathcal{Q}_2.$$

Let $Y_i^1 = J(X_i^1)$ and $Y_i^2 = J(X_i^2)$, $i = 1, \dots, n$ be the image samples in \mathcal{S}^{k-1} . Also, we denote $\bar{Y}_n^1 = \frac{1}{n} \sum_{i=1}^n Y_i^1$ and $\bar{Y}_n^2 = \frac{1}{n} \sum_{i=1}^n Y_i^2$ the corresponding sample means. Let $\mu_{\tilde{\mathcal{Q}}_1}$ and $\mu_{\tilde{\mathcal{Q}}_2}$ be the means of $\tilde{\mathcal{Q}}_1 = \mathcal{Q}_1 \circ J^{-1}$ and $\tilde{\mathcal{Q}}_2 = \mathcal{Q}_2 \circ J^{-1}$, and G^1 and G^2 be the random matrices with the limit distributions of $G_n^1 = \sqrt{n}(\bar{Y}_n^1 - \mu_{\tilde{\mathcal{Q}}_1})$ and $G_n^2 = \sqrt{n}(\bar{Y}_n^2 - \mu_{\tilde{\mathcal{Q}}_2})$, respectively.

Following the standard two-sample hypothesis procedure (see e.g., [19]), which was also used in [3], we are able to construct the test statistic by comparing the means $\mu_{\tilde{\mathcal{Q}}_1}$ and $\mu_{\tilde{\mathcal{Q}}_2}$. Therefore, if the null hypothesis H_0 is true, then we have $\mu_{\tilde{\mathcal{Q}}_1} = \mu_{\tilde{\mathcal{Q}}_2} = \mu$. Then, by the independence assumption of \mathcal{Q}_1 and \mathcal{Q}_2 , we know from Theorem 1 that

$$\begin{aligned} & \sqrt{2n} \left(\Pi_{\mathcal{S}_+^{k-1}(m)}(\bar{Y}_n^1) - \Pi_{\mathcal{S}_+^{k-1}(m)}(\bar{Y}_n^2) \right) \\ &= \sqrt{2n} \left(\Pi_{\mathcal{S}_+^{k-1}(m)}(\bar{Y}_n^1) - \Pi_{\mathcal{S}_+^{k-1}(m)}(\mu) \right) - \sqrt{n} \left(\Pi_{\mathcal{S}_+^{k-1}(m)}(\bar{Y}_n^2) - \Pi_{\mathcal{S}_+^{k-1}(m)}(\mu) \right) \\ & \xrightarrow{d} \mathcal{N}\left(0, \frac{1}{2}\Sigma_1 + \frac{1}{2}\Sigma_2\right), \end{aligned}$$

where Σ_1 and Σ_2 are the covariance matrices of the symmetric Gaussian random matrices G^1 and G^2 under some basis of \mathcal{S}^{k-1} . Here, for simplicity, we just choose the standard orthogonal basis of \mathcal{S}^{k-1} , i.e.,

$$\left\{ e_i e_i^T, \frac{1}{2}(e_i e_j^T + e_j e_i^T) \mid 1 \leq i < j \leq k-1 \right\}, \quad (16)$$

and e_i is the vector with the i -th entry being one and the others being zeros. We use the pooled sample mean $\bar{\mu}_n := \frac{\bar{Y}_n^1 + \bar{Y}_n^2}{2}$ to estimate the true mean μ . Also, let $S^1, S^2 \in \mathbb{R}^{(k-1) \times n}$ be two matrices whose j -th columns are the coordinate vectors of $\Pi'_{\mathcal{S}_+^{k-1}(m)}(\bar{\mu}_n)(Y_j^1 - \bar{\mu}_n)$ and $\Pi'_{\mathcal{S}_+^{k-1}(m)}(\bar{\mu}_n)(Y_j^2 - \bar{\mu}_n)$ under the standard basis of \mathcal{S}^{k-1} given by (16), respectively. Denote $\bar{\Sigma}_1$ and $\bar{\Sigma}_2$ the sample covariance matrices of the random vector $\{S_j^1\}_{j=1}^n$ and $\{S_j^2\}_{j=1}^n$, respectively. Finally, we define the statistic

$$T := (S^1 - S^2)^T \left(\frac{1}{n}\bar{\Sigma}_1 + \frac{1}{n}\bar{\Sigma}_2 \right)^{-1} (S^1 - S^2).$$

If we know that the H_0 is true, then T converges in distribution to χ^2 distribution with $d := \frac{(k-1)(k-2)}{2}$ degrees of freedom. Therefore, we will reject H_0 at asymptotic level τ if

$$T > \chi_d^2(1 - \tau),$$

where $\chi_d^2(1 - \tau)$ is the $(1 - \tau)$ -quantile of the Chi-squared distribution with d degrees of freedom.

Next, we will implement the obtained statistical test of the reflection shapes on the following simple classification problem taken from [13]. We will use the exact same settings as those of [13]

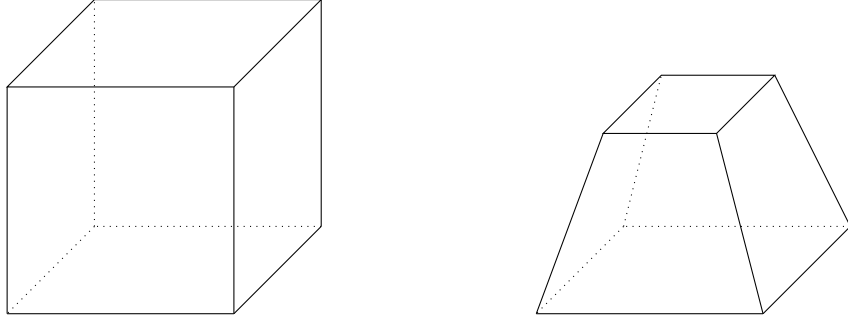


Figure 1: The classification of the cube and pyramid

in the numerical expression. Consider two 3D-shapes in Figure 1: the left one is the regular unit cube and the right one is the pyramids without top section. Each one has 8 landmarks. With different parameters $\varepsilon > 0$, two configurations in Figure 1 can be represented by the following 3×8 matrices ($\varepsilon = 1$ for the left one and $0 < \varepsilon < 1$ for the right one)

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

Also, we add independent Gaussian noise with mean 0 and variance $\sigma^2 = 0.2$ to each landmark. For each shape, let the sample size $n = 10$. We try to distinguish these two shapes by considering the test for the equality of means to the significance level 0.05. We report the percentages of correct classifications as follows.

Table 1: Percentage of correct classification in 1000 simulations

| ε | Z-mean | D-mean | S-mean | E-mean |
|---------------|--------|--------|--------|--------|
| 0 | 74% | 20% | 40% | 70% |
| 0.2 | 57% | 15% | 31% | 62% |
| 0.3 | 42% | 10% | 21% | 59% |

In Table 1, our extrinsic mean of reflection shapes is denoted by “E-mean”. The Ziezold mean (cf. [13]), the mean defined by Dryden et al. [11] and the Schoenberg mean defined by [3] are denoted by “Z-mean”, “D-mean” and “S-mean”, respectively. The numerical results of the Z-mean are taken from [13]. Also, the corresponding R-package can be found from [14]. We implemented our algorithms for the “D-mean”, “S-mean” and “E-mean” in MATLAB 2013a. The numerical experiments were run in MATLAB under a Windows 8 64-bit system on an Intel Core i7 2.4GHz CPU with 8GB memory. From Table 1, we can see that in most cases, the performance of the extrinsic reflection shape mean is better than others with respect to the percentage of correct classifications. However, in the case that $\varepsilon = 0$, for the noisy nearly two-dimensional pyramids, the corresponding Schoenberg mean (if exists) and D-mean are always in three-dimensional space. Therefore, the performance of these two means are not as well as others (see also [13] for more details). In particular, we know from the definition of the projections (12) that our extrinsic reflection shape mean may have lower embedding dimension. It can be seen from Table 1 that our extrinsic reflection shape mean performs equally well as the Ziezold mean, where the true embedding dimension is used.

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