



# Nonparametric inference for extrinsic means on size-and-(reflection)-shape manifolds with applications in medical imaging

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## ABSTRACT

For all  $p > 2$ ,  $k > p$ , a size-and-reflection-shape space  $SR\Sigma_{p,0}^k$  of  $k$ -ads in general position in  $\mathbb{R}^p$ , invariant under translation, rotation and reflection, is shown to be a smooth manifold and is equivariantly embedded in a space of symmetric matrices, allowing a nonparametric statistical analysis based on extrinsic means. Equivariant embeddings are also given for the reflection-shape-manifold  $R\Sigma_{p,0}^k$ , a space of orbits of scaled  $k$ -ads in general position under the group of isometries of  $\mathbb{R}^p$ , providing a methodology for statistical analysis of three-dimensional images and a resolution of the mathematical problems inherent in the use of the Kendall shape spaces in  $p$ -dimensions,  $p > 2$ . The Veronese embedding of the planar Kendall shape manifold  $\Sigma_2^k$  is extended to an equivariant embedding of the size-and-shape manifold  $S\Sigma_2^k$ , which is useful in the analysis of size-and-shape. Four medical imaging applications are provided to illustrate the theory.

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## 1. Introduction

This article is concerned with nonparametric statistical analysis of landmark based size-and-shape data and shape data in which each observation  $\mathbf{x} = (x^1, \dots, x^k)$  consists of  $k > p$  points in  $p$  dimension, called a  $k$ -ad, representing  $k$  locations on an object. The choice of landmarks is generally made with expert help in the particular field of application. The objects of study can be anything for which two  $k$ -ads are deemed equivalent modulo a group  $G$  of transformations depending on the features one wishes to compare and the method of collecting and recording of data. As an example, one may consider the problem of discriminating between distributions of images of a normal and a diseased human organ. Here one may or may not discard the effects of magnification and differences that may arise because of variation in size or in equipment used or due to the manner in which images are taken and digitally recorded. An appropriate  $G$  in this case would be the group of direct isometries, if size is taken into account, or the one generated by direct isometries and scaling, as proposed in a pioneering paper by Kendall [1] for measuring shapes, if the size is ignored. To be specific, one considers only  $k$ -ads in which

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the  $k$  points are not all equal, and removes translation by centering the  $k$ -ad  $\mathbf{x} = (x^1, \dots, x^k)$  to

$$\begin{aligned}\xi &= (\xi^1, \dots, \xi^k) \\ \xi^j &= x^j - \bar{x}, \quad \forall j = 1, \dots, k.\end{aligned}\tag{1}$$

Note that the set of all centered  $k$ -ads lie in a vector subspace  $L_k^p$  in  $(\mathbb{R}^p)^k$  of dimension  $pk - p$ ,  $L_k^p = \{\xi = (\xi^1, \dots, \xi^k) \in (\mathbb{R}^p)^k : \xi^1 + \dots + \xi^k = 0\}$ , and,  $L_k^{p*} = L_k^p \setminus \{0\}$ . The size-and-shape  $[\mathbf{x}]_S$  is the equivalence class, or orbit, of  $\xi = (\xi^1, \dots, \xi^k)$  under rotations [2, pp. 57]. If the size is not relevant, its effect is removed by scaling  $\xi$  to unit size as

$$\mathbf{u} = \frac{\xi}{|\xi|}.\tag{2}$$

The transformed quantity  $\mathbf{u}$  is called a *preshape*, and the set  $S(L_k^{p*})$  of all preshapes comprises a manifold of dimension  $pk - p - 1$ , namely, the unit sphere in  $L_k^p$  called the *preshape sphere*. Note that  $S(L_k^{p*}) \sim S^{pk-p-1}$ , the unit sphere centered at the origin in  $\mathbb{R}^{pk-p}$ . Finally, the *shape*  $[\mathbf{x}]$  of this  $k$ -ad is defined to be the orbit, of  $\mathbf{u} = (u^1, \dots, u^k)$  under all rotations in  $\mathbb{R}^p$  [2, pp. 56–57]. That is,

$$\begin{aligned}[\mathbf{x}]_S &= \{A\xi = (A\xi^1, \dots, A\xi^k) : A \in SO(p)\}, \\ [\mathbf{x}] &= \{A\mathbf{u} = (Au^1, \dots, Au^k) : A \in SO(p)\},\end{aligned}\tag{3}$$

where  $SO(p)$  is the *special orthogonal group* of all  $p \times p$  matrices  $A$  such that  $A^T A = I_p$ ,  $\text{Det}(A) = 1$ . Thus the  $p$ -dimensional size-and-shape-space is  $S\Sigma_p^k = L_k^{p*}/SO(p) \sim (\mathbb{R}^{pk-p} \setminus \{0\})/SO(p)$  and the *Kendall shape space* or the *similarity shape space* is the compact quotient space  $\Sigma_p^k = S(L_k^{p*})/SO(p) \sim S^{pk-p-1}/SO(p)$ .

Under the quotient topology,  $\Sigma_2^k \sim \mathbb{S}^{2k-3}/SO(2)$ , is a compact differentiable manifold of dimension  $2k - 4$ . A convenient representation of Kendall shape space  $\Sigma_2^k$  is achieved by regarding each planar  $k$ -ad as an ordered set of  $k$  complex numbers  $\mathbf{x} = (x^1, \dots, x^k)$ . The Kendall shape  $[\mathbf{x}]$  of the  $k$ -ad  $\mathbf{x}$ , represented by the orbit under rotations ( $SO(2) \sim S^1$ ) of the preshape  $\mathbf{u}$ , is in a one-to-one correspondence with  $SO(2)$ , namely,

$$[\mathbf{x}] = \{e^{i\theta} \mathbf{u} : -\pi < \theta \leq \pi\},\tag{4}$$

which is a point on  $\mathbb{CP}(L_k^2)$ , projective space of the complex vector space  $L_k^2$  of complex dimension  $k - 1$ .

Unfortunately, for  $p > 2$  (and in particular  $p = 3$ ), both  $S\Sigma_p^k = L_k^{p*}/SO(p)$  and  $\Sigma_p^k = S(L_k^{p*})/SO(p)$  have singularities, due to the fact that the actions of  $SO(p)$  on  $\mathbb{R}^{pk-p} \setminus \{0\}$ , and on  $S^{pk-p-1}$  are not *free*, i.e., there are  $k$ -ads  $\mathbf{x}$  for which there exist different  $A, B$  in  $SO(p)$  such that  $A\mathbf{u} = B\mathbf{u}$  (in the representation (2)), so that the orbits of  $\xi$ , respectively of  $\mathbf{u}$ , and  $SO(p)$  are in general not one-to-one. For  $p = 3$ , this is the case if the  $k$  landmarks of a  $k$ -ad are collinear so that the  $k$  points in the preshape  $\mathbf{u}$  lie on a straight line; note that  $\xi$ , respectively  $\mathbf{u}$ , are left invariant by the nontrivial subgroup of rotations around this line as axis. The orbits of  $S\Sigma_p^k$ , respectively of  $\Sigma_p^k$ , are of different dimensions in different regions, thus failing to be differentiable manifolds in the usual sense. The existence of singularities has been a well-recognized problem since the inception of the Kendall theory [3,4]. This impedes the statistical analysis of three-dimensional images, if one adheres to Kendall shape spaces.

It is a main focus of this article (a) to provide (in Section 3) an alternate, but analogous, notion of a higher-dimensional size-and-shape space and of a shape space which are smooth differentiable manifolds, and (b) to construct (in Section 4) *equivariant embeddings* of these manifolds into vector spaces of matrices, using an important representation of Schoenberg [5] relating an *Euclidean distance matrix* of squared inter-point distances of a set of  $k$  points in  $\mathbb{R}^p$  and the  $k \times k$  positive semidefinite matrix of the inner products of the corresponding centered points, which is for size-and-shapes. Using a  $\mathcal{G}$ -equivariant embedding of a manifold  $M$  we will simply mean here that a group  $\mathcal{G}$  of transformations of  $M$  are restrictions of transformations of that group on the ambient space. If the group  $\mathcal{G}$  is relatively large, the embedding preserves many symmetries of the manifold  $M$ . It is then appropriate to apply the general nonparametric theory in Bhattacharya and Patrangenaru [6,7]. The *size-and-reflection-shape*  $[\mathbf{x}]_{RS}$  of the  $k$ -ad  $\mathbf{x}$  and the *reflection-shape*  $[\mathbf{x}]_R$  of this  $k$ -ad, are, respectively, the  $O(p)$ -orbit of the centered configuration  $\xi$ , and of the preshape  $\mathbf{u}$  under the action  $A\xi = (A\xi^1, \dots, A\xi^k)$  of the orthogonal group  $O(p)$  (of  $p \times p$  matrices  $A$  satisfying  $A^T A = I_p$ ) on the set of all centered  $k$ -ads [2, p. 57]. Thus

$$[\mathbf{x}]_{RS} = \{A\xi : A \in O(p)\}, \quad [\mathbf{x}]_R = \{A\mathbf{u} : A \in O(p)\}.\tag{5}$$

The set of all size-and-reflection-shapes (respectively, reflection shapes) of  $k$ -ads in *general position*  $\xi$ , i.e.  $k$ -ads for which  $\{\xi^1, \dots, \xi^k\}$  spans  $\mathbb{R}^p$ , is the *size-and-reflection-shape space*  $SR\Sigma_{p,0}^k$  (respectively, the *reflection-shape space*  $\Sigma_{p,0}^k$ ). Both these spaces are manifolds, since the action of an orthogonal matrix on  $\mathbb{R}^p$  is uniquely determined by its action on a basis of  $\mathbb{R}^p$ , and a centered  $k$ -ad in general position includes such a basis.

A first approach to size-and-shape analysis using a Euclidean distance matrix, which differs from ours, is due to Lele [8]. The manifold approach to reflection-shape analysis, including Schoenberg embeddings and connections to *multidimensional scaling* (MDS), was initiated by Bandulasiri and Patrangenaru [9]. A mean reflection shape, introduced by Dryden et al. [10], which is called here *MDS mean reflection shape* is not an extrinsic mean, as recently pointed out in Section 5 and by

Bhattacharya [11]. For this reason the manifold based reflection-shape analysis approach in our paper has very limited connection with the MDS based mean reflection-shape estimators in [2, p. 281]. In Section 5 we also introduce the Schoenberg embedding of the size-and-reflection-shape manifold  $S\Sigma_{p,0}^k$ . The extrinsic sample mean size-and-reflection-shape under this embedding turns out to be the sample estimate  $[MDS_p(W)]_{RS}$  in [2, p. 281]. However, the population mean defined by the latter (see [2, pp. 88, 279]), in the parametric or semiparametric setting, is in general different from the extrinsic mean in the present work, unless the underlying distribution has additional structure (such as isotropy, in the case  $p = 2$ ). It now follows from the general results on the consistency of the extrinsic sample mean as an estimator of the extrinsic mean (see Bhattacharya and Patrangenaru [6]) that the estimate in Dryden and Mardia [2] is a consistent estimate of their target population parameter only for certain special classes of distributions.

Section 5 provides the main ingredients for asymptotic nonparametric inference based on Schoenberg means on  $S\Sigma_{p,0}^k$  and  $\Sigma_{p,0}^k$ . The necessary and sufficient condition for a probability measure  $Q$  on  $S\Sigma_{p,0}^k$  or on  $\Sigma_{p,0}^k$  to be Schoenberg-nonfocal is that, in their decreasing order, the eigenvalues of rank  $p$  and  $p + 1$  of the mean matrix of the push forward distribution are distinct. Although on  $\Sigma_{p,0}^k$  this condition is the same as that for the existence of an MDS mean in Dryden et al. [10], the extrinsic mean differs from the MDS mean in Dryden et al. [10], and from the MDS sample mean estimate in Dryden and Mardia [2] or in Kent [12] (in the case  $p = 2$ ).

A second result of significance is the identification of space  $S\Sigma_2^k$  of size-and-shapes  $[\mathbf{x}]_S$  of planar  $k$ -ads  $\mathbf{x}$ ,

$$[\mathbf{x}]_S = \{w\xi : w \in \mathbb{C}, |w| = 1\}, \quad (6)$$

with a noncompact manifold—direct product of  $\Sigma_2^k$  and  $(0, \infty)$ . In Section 4, an equivariant embedding  $\phi$  of the planar size-and-shape manifold  $S\Sigma_2^k$ , extending the Veronese Whitney embedding of the Kendall shape space in Bhattacharya and Patrangenaru [6], is given. In Section 5 one shows that the extrinsic mean size-and-shape of a probability measure  $Q$  on  $S\Sigma_2^k$  exists (i.e.  $Q$  is  $\phi$ -nonfocal) if and only if the largest eigenvalue  $\lambda_k$  of the push forward probability measure  $\phi(Q) = Q \circ \phi^{-1}$  is simple, and in this case the extrinsic mean size-and-shape is  $[\lambda_k \mathbf{u}_0]_S$ , where  $\mathbf{u}_0$  is a unit eigenvector of the mean matrix  $\tilde{\mu}$  of  $Q \circ \phi^{-1}$ . This provides a proper venue for a future study of *allometry*—the dependence of shape on size, in various contexts.

Finally, Section 7 illustrates the theory by applications with real data. We give a high-dimensional example of extrinsic sample mean reflection-size-and-shape of protein structures from the same family of proteins which are posted on the Protein Data bank (PDB). In the next example, on glaucoma detection, one analyzes paired samples valued in the three-dimensional size-and-reflection-shape space  $S\Sigma_{p,0}^k$  with  $p = 3, k = 4$ . The dimension of this flat manifold is 6. Simultaneous bootstrapped Bonferroni confidence regions are constructed for the means of six Euclidean coordinates in order to test the presence of the treatment effect (size-and-reflection-shape change due to glaucoma). Discrimination based on size-and-shape (rather than shape alone) is appropriate for such matched pair data, since a size change of the eyecup may very well be induced by glaucoma. Because the sample size 12 is rather small for dealing with six-dimensional data, bootstrapping is preferred over classical asymptotics. Individual coordinates are used in order to identify specific shape features leading to significance. In a second example one shows that there is a significant difference between mean planar similarity shapes of mid-face cranial configurations between Apert syndrome children and healthy children. Another application is for the estimation of mean size-and-shape of a two-dimensional image of a section of the skull of a group of healthy children.

## 2. Planar size-and-shape manifolds

Consider  $k$ -ads,  $k > 2$ , with  $k$  points in the plane, not all the same. A manifold of interest in shape analysis is the planar size-and-shape space  $S\Sigma_2^k$  (see [2, p. 57]). Two planar  $k$ -ads have the same size-and-shape if they differ by a direct isometry of the Euclidean plane (a roto-translation). Translate a  $k$ -ad  $\mathbf{x}$  by  $-\bar{\mathbf{x}}$  (i.e. center  $\mathbf{x}$ ) to get a  $k$ -ad  $\xi = (\xi^1, \dots, \xi^k) \in L_k^2$  given by (1). Two  $k$ -ads  $\mathbf{x}, \mathbf{x}'$  have the same direct similarity size-and-shape if there is a  $w \in \mathbb{S}^1 = \{\mathbb{C}, |\mathbf{u}| = 1\}$ , such that  $\xi' = w\xi$ , where  $\xi, \xi' \in L_k^2$  are the centered  $\mathbf{x}, \mathbf{x}'$  respectively. Let  $[\mathbf{x}]_S, [\mathbf{x}]$  and  $r(\mathbf{x})$  be the size-and-shape, shape, and size of  $\mathbf{x}$ , respectively, where  $r^2(\mathbf{x}) = \sum_{i=1}^k |\xi^i|^2$ . Define the one-to-one map  $\psi : S\Sigma_2^k \rightarrow (0, \infty) \times \Sigma_2^k$  given by

$$\psi([\mathbf{x}]_S) = (r(\mathbf{x}), [\mathbf{x}]). \quad (7)$$

The following result is then clear from the discussion in the Introduction on Kendall shape space  $\Sigma_2^k$ .

**Theorem 2.1.** *The planar size-and-shape space  $S\Sigma_2^k$  can be identified with  $(0, \infty) \times \Sigma_2^k$ , a differentiable manifold of dimension  $2k - 3$ .*

In the representation (7), the second coordinate on the right side is the planar similarity shape of a  $k$ -ad, thus allowing a natural mathematical modeling for the change in shape with size growth.

## 3. Reflection-shape manifolds and size-and-reflection-shape manifolds in higher dimensions

A comprehensive account of Kendall shape spaces in arbitrary dimensions can be found in Kendall et al. [3]. Unlike planar direct similarity shape spaces, in dimension  $p \geq 3$  the Kendall shape space  $\Sigma_p^k$  has singularities and no equivariant

embedding of it is known. It is therefore useful and easier to study shapes of configurations with respect to the full group of similarities. This group,  $\text{Sim}(p)$ , is the set of transformations of the Euclidean space  $\mathbb{R}^p$ , of the form

$$\mathbf{x}' = B\mathbf{x} + b, \quad B^T B = cI_p, \quad c > 0. \quad (8)$$

The reflection shape  $[\mathbf{x}]_R$  of a  $k$ -ad  $\mathbf{x}$ , which is regarded here as a  $p$  by  $k$  matrix, is defined by (5). The reflection-shape manifold, introduced in Section 1, then is the set

$$R\Sigma_{p,0}^k = \{[\mathbf{x}]_R, \mathbf{x} \text{ in general position}\} = \{[\mathbf{x}]_R, \text{rk } \mathbf{x} = p\} \quad (9)$$

where  $\text{rk } \mathbf{x}$  is the rank of  $\mathbf{x}$ . The manifold dimension, codimension of the  $O(p)$ -orbits in  $(\mathbb{R}^p)^k$ , is  $\dim \Sigma_{p,0}^k = kp - \frac{p(p+1)}{2} - 1$ .

The size-and-reflection-shape  $[\mathbf{x}]_{RS}$  of a  $k$ -ad  $\mathbf{x}$  in  $\mathbb{R}^p$  is defined in (5), and the size-and-reflection-shape space  $S\Sigma_{p,0}^k$  is the set

$$SR\Sigma_{p,0}^k = \{[\mathbf{x}]_{RS}, \mathbf{x} \text{ in general position}\} = \{[\mathbf{x}]_{RS}, \text{rk } \mathbf{x} = p\}. \quad (10)$$

Recall that, by the fundamental theorem of Euclidean geometry, any isometry of the Euclidean space is a linear transformation of  $\mathbb{R}^p$  of the form

$$\mathbf{x}' = B\mathbf{x} + b, \quad B^T B = I_p, \quad (11)$$

therefore, if one centers the  $k$ -ad  $\mathbf{x}$  to  $\xi = (x^1 - \bar{x}, \dots, x^k - \bar{x}) \in L_k^p$ , then  $[\mathbf{x}]_{RS} = [\xi]_{RS}$ , and if a  $k$ -ad  $\mathbf{x}'$ , having the same reflection shape as  $\mathbf{x}$ , differs from  $\mathbf{x}$  by the isometry (11), then

$$\bar{x}' = B\bar{x} + b. \quad (12)$$

Therefore  $\xi' = B\xi$ , where  $\xi' \in L_k^p$  is obtained by centering the  $k$ -ad  $\mathbf{x}'$ . Thus, if we set  $L_{k,p,0} = \{\xi \in L_k^p, \text{rk } \xi = p\}$ , the manifold  $S\Sigma_{p,0}^k$  can be represented as a quotient  $L_{k,p,0}/O(p)$  and the manifold dimension of  $\Sigma_{p,0}^k$  is  $kp - \frac{p(p+1)}{2}$ .

#### 4. Equivariant embeddings of $\Sigma_2^k$ , $S\Sigma_2^k$ , $R\Sigma_{p,0}^k$ and $RS\Sigma_{p,0}^k$

Recall from Section 1 the complex representation (4) of the direct similarity shape  $\sigma(\mathbf{x})$  of a planar  $k$ -ad  $\mathbf{x}$ . The quadratic Veronese–Whitney embedding of  $\Sigma_2^k$  into  $S(k, \mathbb{C})$ , the linear space of self-adjoint complex matrices of order  $k$ , (or simply the Veronese–Whitney map) is  $j : \Sigma_2^k \rightarrow S(k, \mathbb{C})$ , where with  $\mathbf{u}$  representing the preshape as in (4),

$$j([\mathbf{x}]) = \mathbf{u}\mathbf{u}^*, \quad \mathbf{u}^*\mathbf{u} = 1. \quad (13)$$

Extend (13) to an embedding  $\phi$  of the product model of  $S\Sigma_2^k$  in Theorem 2.1 into  $\mathbb{C}^{k^2}$  (regarded as the set of all  $k \times k$  complex matrices) given by

$$\phi([\mathbf{x}]_S) = r\mathbf{u}\mathbf{u}^*, \quad r > 0, \mathbf{u} \in L_k, \mathbf{u}^*\mathbf{u} = 1. \quad (14)$$

Note that the range of  $\phi$  in (14) is a closed noncompact submanifold of  $S(k, \mathbb{C})$ .

The distance  $\rho$  on  $S\Sigma_2^k$  is the Euclidean distance inherited from the embedding  $\phi$ .

The embedding  $\phi$  (as well as  $j$ ) is  $\mathcal{G}$ -equivariant, where  $\mathcal{G}$  is isomorphic to the group  $SU(k-1)$  of  $(k-1) \times (k-1)$  unitary matrices with determinant 1 (see [3,6]).

In higher dimensions, using an approach based on the well-known result in multidimensional scaling (MDS) (see [5, 13], [14, p. 397]), Bandulasiri and Patrangenaru [9] introduced the Schoenberg embedding of reflection shapes in higher dimensions. Let  $D = (d_{rs})_{r,s=1,\dots,k}$  be a distance matrix between  $k$  points and consider  $A$  and  $B$  defined by  $A = (a_{rs})$ ,  $a_{rs} = -\frac{1}{2}d_{rs}^2$ ,  $\forall r, \forall s = 1, \dots, k$ ,  $B = \tilde{H}A\tilde{H}^T$ , where  $\tilde{H} = I_k - k^{-1}\mathbf{1}_k\mathbf{1}_k^T$  is the centering matrix in  $\mathbb{R}^k$ . A version of the Schoenberg theorem suitable for our purposes is given below. Theorem 4.1 is an edited version of Theorem 14.2.1 in Mardia et al. [14, pp. 397–398].

**Theorem 4.1.** (a) If  $D$  is a matrix of Euclidean distances  $d_{rs} = \|\mathbf{x}^r - \mathbf{x}^s\|$ ,  $\mathbf{x}^j \in \mathbb{R}^p$ , and we set  $X = (\mathbf{x}^1 \dots \mathbf{x}^k)^T$ ,  $k > p$ , then  $B$  is given by

$$b_{rs} = (\mathbf{x}^r - \bar{\mathbf{x}})^T (\mathbf{x}^s - \bar{\mathbf{x}}), \quad r, s = 1, \dots, k. \quad (15)$$

In matrix form,  $B = (\tilde{H}X)(\tilde{H}X)^T$ .

(b) Conversely, assume that  $B$  is a  $k \times k$  symmetric positive semidefinite matrix  $B$  of rank  $p$ , having zero row sums. Then  $B$  is a centered inner product matrix for a configuration  $X$  constructed as follows. Let  $\lambda_1 \geq \dots \geq \lambda_p$  denote the positive eigenvalues of  $B$  with corresponding eigenvectors  $\mathbf{x}_{(1)}, \dots, \mathbf{x}_{(p)}$  normalized by

$$\mathbf{x}_{(i)}^T \mathbf{x}_{(i)} = \lambda_i. \quad (16)$$

Then the  $k$  points  $P_r \in \mathbb{R}^p$  with coordinates  $\mathbf{x}^r = (x_{r1}, \dots, x_{rp})^T$ ,  $r = 1, \dots, k$ , where  $\mathbf{x}^r$  is the  $r$ th row of the  $k \times p$  matrix  $(\mathbf{x}_{(1)} \dots \mathbf{x}_{(p)})$ , have center  $\bar{\mathbf{x}} = 0$ , and  $B = \tilde{H}A\tilde{H}^T$  where  $A = -\frac{1}{2}(\|\mathbf{x}^r - \mathbf{x}^s\|^2)_{r,s=1,\dots,k}$ .

Let  $S(k, \mathbb{R})$  denote the set of all  $k \times k$  real symmetric matrices. The Schoenberg embedding  $J : R\Sigma_{p,0}^k \rightarrow S(k, \mathbb{R})$  is given by:

$$A = J([\mathbf{x}]_R) = \mathbf{u}^T \mathbf{u}, \quad (17)$$

where  $\mathbf{u} = \xi / \|\xi\|$  and  $\xi = (x^1 - \bar{x}, \dots, x^k - \bar{x}) \in (\mathbb{R}^p)^k$  identified with  $\mathcal{M}(p, k; \mathbb{R})$ . Since  $J$  is differentiable, to show that  $J$  is an embedding it suffices to show that  $J$  and its derivative are both one-to-one. If  $J([\mathbf{x}]_R) = J([\mathbf{x}']_R)$ , from (17) the Euclidean distances between corresponding landmarks of the scaled configurations are equal

$$\|u^i - u^j\| = \|u'^i - u'^j\|, \quad \forall i, j = 1, \dots, k. \quad (18)$$

Moreover since  $\sum_{i=1}^k u^i = \sum_{i=1}^k u'^i = 0$ , by the fundamental theorem of Euclidean geometry, there is a matrix  $T \in O(p)$  such that  $u'^i = Tu^i$ ,  $\forall i = 1, \dots, k$ . If we set  $B = \frac{\|\xi\|}{\|\xi'\|} T$ ,  $b = \bar{x}' - B\bar{x}$ , it follows that  $x'^i = Bx^i + b$ ,  $\forall i = 1, \dots, k$  with  $B^T B = cI_p$ , and from (8), we see that  $[\mathbf{x}]_R = [\mathbf{x}']_R$ . Thus  $J$  is one-to-one. The proof of the injectivity of the derivative of  $J$  is left to the reader.

**Theorem 4.2.** *The range of the Schoenberg embedding of  $R\Sigma_{p,0}^k$  is the subset  $M_{k,p}$  of  $k \times k$  positive semidefinite symmetric matrices  $A$  with  $\text{rk} A = p$ ,  $A\mathbf{1}_k = 0$ ,  $\text{Tr} A = 1$ , where  $\mathbf{1}_k$  is the  $k \times 1$  column vector  $(1 \dots 1)^T$ .*

The proof is a straightforward application of Theorem 4.1.

The Schoenberg embedding of the size-and-reflection-shape manifold is  $J : SR\Sigma_{p,0}^k \rightarrow S(k, \mathbb{R})$ , given by

$$J([\xi]_{RS}) = \xi^T \xi. \quad (19)$$

The following result will be used to derive formulas for extrinsic parameters and for their estimators.

**Theorem 4.3.** *The range of the Schoenberg embedding of  $SR\Sigma_{p,0}^k$  is the subset  $SM_{k,p}$  of  $k \times k$  positive semidefinite symmetric matrices  $A$  with  $\text{rk} A = p$ ,  $A\mathbf{1}_k = 0$ .*

The proof is similar to the proof of Theorem 4.2.

Consider a  $(k-1) \times k$  matrix  $H$ , whose rows are all of unit length, orthogonal to each other and orthogonal to the row vector  $\mathbf{1}_k^T$ .

**Proposition 4.1.** *Let  $M_k$  be the space of  $k \times k$  symmetric matrices  $A$  with  $A\mathbf{1}_k = 0$ . The map  $\phi$  from  $M_k$  to  $S(k-1, \mathbb{R})$ , given by  $\phi(A) = \mathbf{H}A\mathbf{H}^T$  is an isometry. In addition,  $\text{Tr}(\phi(A)) = \text{Tr}(A)$ .*

**Proof.** Since  $\phi$  in Proposition 4.1 is a linear map, it suffices to show that  $\|\phi(A)\| = \|A\|$ . Here we consider the Euclidean norm of a matrix  $M$  given by  $\|M\|^2 = \text{Tr}(MM^T)$ . The claims are easily verified from the relations  $\mathbf{H}\mathbf{H}^T = \mathbf{I}_{k-1}$ ,  $\mathbf{H}\mathbf{H} = \mathbf{I}_k - \frac{1}{k}\mathbf{1}_k\mathbf{1}_k^T$ , and the fact that for any matrices  $A, B$ ,  $\text{Tr}(AB) = \text{Tr}(BA)$ , whenever both products make sense. ■

We may then define an embedding  $\psi$  of the size-and-reflection-shape manifold as  $\psi : SR\Sigma_{p,0}^k \rightarrow S(k-1, \mathbb{R})$ , given by

$$\psi([\xi]_R) = \mathbf{H}\xi^T \xi \mathbf{H}^T. \quad (20)$$

From Proposition 4.1 it follows that the Schoenberg embedding and the embedding  $\psi$  induce the same distance on  $SR\Sigma_{p,0}^k$ .

**Remark 4.1.** The range of  $\psi$  is the set of  $(k-1) \times (k-1)$  symmetric matrices of rank  $p$ . Note that for  $k = p+1$ , the range is the open convex subset  $S_+(k-1, \mathbb{R}) \subset S(k-1, \mathbb{R})$  of positive definite symmetric matrices and the induced distance on  $SR\Sigma_{p,0}^k$  is a Euclidean distance.

**Remark 4.2.** Let  $O(k)$  act on  $SR\Sigma_{p,0}^k$  as  $([\xi]_{RS}, A) \rightarrow [\xi A]_{RS}$ ,  $A \in O(k)$ . Then the embedding (19) is  $O(k)$ -equivariant. This action is not free. But in view of Proposition 4.1, the Schoenberg embedding can be “tightened” to an  $O(k-1)$ -equivariant embedding in  $S(k-1, \mathbb{R})$ .

## 5. Extrinsic means and their estimators

We recall from Bhattacharya and Patrangenaru [6] that the extrinsic mean  $\mu_{J,E}(Q)$  of a nonfocal probability measure  $Q$  on a manifold  $M$  w.r.t. an embedding  $J : M \rightarrow \mathbb{R}^N$ , when there exists, is the point from which the expected squared (induced Euclidean) distance under  $Q$  is minimum. It is given by  $\mu_{J,E}(Q) = J^{-1}(P_J(\mu))$ , where  $\mu$  is the usual mean of  $J(Q)$  as a probability measure on  $\mathbb{R}^N$  and  $P_J$  is its projection on  $J(M)$  [6, Proposition 3.1]. When the embedding  $J$  is given, and the projection  $P_J(\mu)$  is unique, one often identifies  $\mu_{J,E}$  with its image  $P_J(\mu)$ , and refer to the latter as the extrinsic mean. The term “nonfocal  $Q$ ” means that the projection (minimizer of the distance from  $\mu$  to points in  $J(M)$ ) is unique. Often the extrinsic mean will be denoted by  $\mu_E(Q)$ , or simply  $\mu_E$ , when  $J$  and  $Q$  are fixed in a particular context.

Assume that  $(X_1, \dots, X_n)$  are i.i.d.  $M$ -valued random objects whose common probability measure is  $Q$ , and let  $\bar{X}_E := \mu_{J,E}(\hat{Q}_n) = \mu_E(\hat{Q}_n)$  be the extrinsic sample mean. Here  $\hat{Q}_n = \frac{1}{n} \sum_{j=1}^n \delta_{X_j}$  is the empirical distribution.

In this section we will consider extrinsic means associated with embeddings of the four types of manifolds described in Section 4.

### 5.1. Mean planar shape and mean planar size-and-shape

We first describe the extrinsic mean of a probability measure  $Q$  on  $\Sigma_2^k$  with respect to the Veronese–Whitney map  $j$  given in (13). The squared distance in the space  $S(k, \mathbb{C})$  of self-adjoint matrices is  $d_0^2(A, B) = \text{Tr}((A - B)(A - B)^*) = \text{Tr}((A - B)^2)$ .

A probability measure  $Q$  on  $\Sigma_2^k$  may be viewed as a distribution of a random shape  $[\mathbf{U}]$ , where  $\mathbf{U}$  is a random preshape (see (3) and (4)). This probability measure  $Q$  is  $J$ -nonfocal if the largest eigenvalue of  $E(\mathbf{U}\mathbf{U}^*)$  is simple, and in this case  $\mu_{J,E}(Q) = [\mu]$ , where  $\mu \in S(L_k^2)$  is a unit eigenvector corresponding to this largest eigenvalue (see Bhattacharya and Patrangenaru [6]).

The extrinsic sample mean direct similarity planar shape  $[\overline{\mathbf{X}}]_{J,E}$  of a random sample  $[\mathbf{X}_r]$  with preshapes  $\mathbf{U}_r = [U_r^1 : \dots : U_r^k]$ ,  $\mathbf{1}_k^T \mathbf{U}_r = 0$ ,  $\|\mathbf{U}_r\| = 1$ ,  $r = 1, \dots, n$ , from such a nonfocal distribution exists with probability converging to 1 as  $n \rightarrow \infty$  (see [6]) and is given by

$$[\overline{\mathbf{X}}]_{J,E} = [\mathbf{U}], \quad (21)$$

where  $\mathbf{U}$  is a unit eigenvector in  $S(L_k^2)$  corresponding to the largest eigenvalue of

$$K := n^{-1} \sum_{r=1}^n \mathbf{U}_r \mathbf{U}_r^*. \quad (22)$$

This means that  $[\overline{\mathbf{X}}]_{J,E}$  is given by a formula that is similar to the one for the *full Procrustes estimate* of the mean shape in parametric families such as Dryden–Mardia type distributions or complex Bingham type distributions for planar shapes on  $\Sigma_2^k$  [15, 12]. For this reason, the Veronese–Whitney extrinsic sample mean shape may be called the *Procrustes* mean estimate.

To compute the extrinsic mean of probability measures on  $S\Sigma_2^k$ , we proceed exactly as in the case of  $\Sigma_2^k$ , but under the additional assumption that the image of  $Q$  under  $\phi$ , namely  $Q \circ \phi^{-1}$ , regarded as a probability measure on  $\mathbb{C}^{k^2} (\approx \mathbb{R}^{2k^2})$  has finite second moments. With this assumption, let  $\tilde{\mu}$  be the mean ( $k \times k$  matrix) of  $\phi(Q) = Q \circ \phi^{-1}$ . Then  $\tilde{\mu}$  is a Hermitian matrix, which is positive semidefinite. There exists a complex orthogonal matrix  $T$  such that  $T\tilde{\mu}T^* = D = \text{diag}(\lambda_1, \dots, \lambda_k)$ , where  $0 \leq \lambda_1 \leq \dots \leq \lambda_k$  are the eigenvalues of  $\tilde{\mu}$ . Then if  $\mathbf{v} = \sqrt{r}T\mathbf{u}$ , the squared distance between  $\tilde{\mu}$  and an element  $\phi([\mathbf{x}]_S)$  of  $\phi(S\Sigma_2^k)$  is given by

$$\begin{aligned} \text{Trace}(\tilde{\mu} - r\mathbf{u}\mathbf{u}^*)^2 &= \text{Trace}(D - \mathbf{v}\mathbf{v}^*)^2 \\ &= \sum_j \lambda_j^2 + \sum_j |v_j|^4 - 2 \sum_j \lambda_j |v_j|^2 + \sum_{j \neq j'} |v_j \bar{v}_{j'}|^2 \\ &= \sum_j \lambda_j^2 + \sum_j |v_j|^4 - 2 \sum_j \lambda_j |v_j|^2 + \sum_j |v_j|^2 \sum_j |v_j'|^2 - \sum_j |v_j|^4 \\ &= \sum_j \lambda_j^2 - 2 \sum_j \lambda_j |v_j|^2 + r^2(\mathbf{x}) \end{aligned} \quad (23)$$

noting that  $|\mathbf{v}|^2 = r(\mathbf{x})$ . We first minimize (23) for a given size  $r = r(\mathbf{z})$ . Clearly this is achieved by letting  $\mathbf{v} = \sqrt{r}e_k$  (or  $\sqrt{r}e^{i\theta}e_k$  for some  $\theta$ ), where  $e_k$  has 1 as its last ( $k$ th) coordinate, and zeros elsewhere. Then  $\mathbf{u} = \frac{1}{\sqrt{r}}T^*\mathbf{v}$  is an eigenvector of  $\tilde{\mu}$  in the eigenspace of the largest eigenvalue  $\lambda_k$ . With this choice (23) becomes

$$\sum_j \lambda_j^2 - 2r\lambda_k + r^2. \quad (24)$$

The minimum of (24) over all  $r > 0$  is attained with  $r = \lambda_k$ . Hence the minimum of (23) is achieved by an element  $\mathbf{u} = \mathbf{u}_0$  where  $\mathbf{u}_0$  is a unit vector in the eigenspace of  $\lambda_k$ , i.e., by the element  $\phi([\mathbf{x}]_S) = \phi([\lambda_k \mathbf{u}_0]_S)$  of  $\phi(S\Sigma_2^k)$ . If  $\lambda_k$  is a simple eigenvalue of  $\tilde{\mu}$ , then this minimizer is *unique*. In this case the extrinsic mean  $\mu_E$  of  $Q$  is the size-and-shape of  $\lambda_k \mathbf{u}_0$ . Hence the consistency theorem in [6] applies in this case. The size of the mean  $\mu_E$  is  $\lambda_k$ .

### 5.2. Extrinsic mean reflection shapes and extrinsic mean size-and-reflection-shapes

We consider now a random  $k$ -ad in general position  $\mathbf{X}$ , centered as  $\mathbf{X}_0 = (X^1 - \bar{X}, \dots, X^k - \bar{X}) \in (\mathbb{R}^p)^k \simeq M(p, k; \mathbb{R})$ , and then scaled to  $U$ :

$$\mathbf{U} = \mathbf{X}_0 / \|\mathbf{X}_0\|. \quad (25)$$

Set

$$C = E(\mathbf{X}_0^T \mathbf{X}_0), \quad B = E(\mathbf{U}^T \mathbf{U}). \quad (26)$$

Obviously  $\text{Tr}(B) = 1$ ,  $B\mathbf{1}_k = 0$ ,  $B \geq 0$  and  $C\mathbf{1}_k = 0$ ,  $C \geq 0$ .



The extrinsic mean size-and-reflection-shape of  $[\mathbf{X}]_{RS}$  exists if  $\text{Tr}(C - \xi^T \xi)^2$  has a unique solution  $\xi \in M(p, k; \mathbb{R})$  up to an orthogonal transformation, with

$$\xi \mathbf{1}_k = 0, \quad \text{rk } \xi = p. \quad (27)$$

That is the same as saying that given  $C$ ,  $\xi$  is a *classical solution* in  $\mathbb{R}^p$  to the MDS problem, as given in [14, p. 408] in terms of the first largest  $p$  eigenvalues of  $C$ . Assume that the eigenvalues of  $C$  in their decreasing order are  $\lambda_1 \geq \dots \geq \lambda_k$ . The classical solution of the MDS problem is *unique* (up to an orthogonal transformation) if  $\lambda_p > \lambda_{p+1}$  and  $\xi^T$  can be taken as the matrix

$$V = (v_1 v_2 \dots v_p), \quad (28)$$

whose columns are orthogonal eigenvectors of  $C$  corresponding to the largest eigenvalues  $\lambda_1 \geq \dots \geq \lambda_p$  of  $C$ , with

$$v_j^T v_j = \lambda_j, \quad \forall j = 1, \dots, p. \quad (29)$$

Since the eigenvectors  $v_1, \dots, v_p$  are linearly independent,  $\text{rk } \xi = p$ . If  $v$  is an eigenvector of  $C$  for the eigenvalue  $\lambda > 0$ , since  $C \mathbf{1}_k = 0$  it follows that  $v \mathbf{1}_k = 0$ . Therefore the classical solution  $\xi$  derived from the eigenvectors (28) satisfies (27). In conclusion we have:

**Theorem 5.1.** Assume that  $C = \sum_{i=1}^k \lambda_i e_i e_i^T$  is the spectral decomposition of  $C = E(\mathbf{X}_0^T \mathbf{X}_0)$ , then the extrinsic mean  $\mu_E$  size-and-reflection-shape exists if and only if  $\lambda_p > \lambda_{p+1}$  and if this is the case,  $\mu_E = [\xi]_{RS}$  where  $\xi^T$  can be taken as the matrix (28) satisfying (29).

From Theorem 5.1 it follows that given  $k$ -ads in general position in  $\mathbb{R}^p$ ,  $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ ,  $\mathbf{x}_j = (x_j^1, \dots, x_j^k)$ ,  $j = 1, \dots, n$ , their extrinsic sample mean size-and-reflection-shape is  $[\bar{\mathbf{x}}]_E = [\hat{\xi}]_{RS}$ , where  $\hat{\xi}$  is the classical solution in  $\mathbb{R}^p$  to the MDS problem for the matrix

$$\hat{C} = \frac{1}{n} \sum_{j=1}^n \xi_j^T \xi_j. \quad (30)$$

Here  $\xi_j$  is the matrix obtained from  $\mathbf{x}_j$  after centering, assuming  $\hat{\lambda}_p > \hat{\lambda}_{p+1}$ . Here  $\hat{\lambda}_1 \geq \dots \geq \hat{\lambda}_k$  are the eigenvalues of  $\hat{C}$ . Indeed, the configuration of the sample mean is given by the eigenvectors corresponding to the  $p$  largest eigenvalues of  $\hat{C}$ .

**Remark 5.1.** From Remark 4.1, in the case  $k = p + 1$ , the projection  $P_\psi$  is the identity map, therefore any distribution  $Q$  is  $\psi$ -nonfocal and  $\psi(\mu_{E,\psi})$  is the mean  $\mu$  of  $\psi(Q)$ .

The formula for the extrinsic mean reflection shape of  $[\mathbf{X}]_R$ , has been very recently found by Bhattacharya [11]. This mean exists if

$$\text{Tr}(B - \mathbf{u}^T \mathbf{u})^2 \quad (31)$$

has a unique minimizer  $\mathbf{u} \in M(p, k; \mathbb{R})$  up to an orthogonal transformation, satisfying the constraints

$$\mathbf{u} \mathbf{1}_k = 0, \quad \text{Tr}(\mathbf{u}^T \mathbf{u}) = 1. \quad (32)$$

**Theorem 5.2** (Abhishek Bhattacharya). Assume that  $B = \sum_{i=1}^k \lambda_i e_i e_i^T$  is the spectral decomposition of  $B$ , then the extrinsic mean reflection shape exists if and only if  $\lambda_p > \lambda_{p+1}$ . If this is this case, then  $\mathbf{u}^T$  can be taken as the matrix

$$V = (v_1 v_2 \dots v_p), \quad (33)$$

whose columns are orthogonal eigenvectors of  $B$  corresponding to the largest eigenvalues  $\lambda_1 \geq \dots \geq \lambda_p$  of  $B$ , with

$$\begin{aligned} \text{(a)} \quad & v_j^T \mathbf{1}_k = 0 \\ & \text{and} \\ \text{(b)} \quad & v_j^T v_j = \lambda_j + \frac{1}{p}(\lambda_{p+1} + \dots + \lambda_k), \quad \forall j = 1, \dots, p. \end{aligned} \quad (34)$$

The result stated above is equivalent to the following proposition.

**Proposition 5.1.** The projection of a positive semidefinite matrix  $B$  on  $M_{k,p}$  is given by  $P_{M_{k,p}} B = VV^T$  where  $V$  is given by (33) and (34).

Rather than using the Schoenberg embedding, Dryden et al. [10] defined a one-to-one function from the space  $\Sigma_{p,+}^k$  of reflection shapes of  $k$ -ads of points that are not all the same, to  $S(k-1, \mathbb{R})$ , whose range  $N_{p,k}$  is the set of positive semidefinite symmetric matrices  $B$  with  $\text{rk}(B) \leq p$ ,  $\text{Tr}(A) = 1$ . Their embedding  $\psi$  is given by

$$\psi([\mathbf{x}]_R) = \mathbf{H}J([\mathbf{x}]_R)\mathbf{H}^T, \quad (35)$$

where  $\mathbf{H}$  is the  $(k-1) \times k$  Helmert submatrix (see [2, p. 34]).

**Remark 5.2.** Note that while the condition in [10] for a random reflection shape to be nonfocal is the same as ours, their mean MDS reflection shape is not the extrinsic mean reflection shape (extrinsic mean under the embedding  $\psi$  stated in Theorem 5.2). Indeed their scaling of the eigenvectors  $v_1, \dots, v_p$  corresponding to the  $p$  largest eigenvalues of  $B$  is given by

$$v_j^T v_j = \frac{\lambda_j}{\lambda_1 + \dots + \lambda_p}, \quad \forall j = 1, \dots, p, \quad (36)$$

and the MDS mean reflection shape is  $\mu_{MDS} = [\mathbf{u}]_R$ .

## 6. Asymptotic distribution of extrinsic sample mean size-and-reflection-shapes

The reflection shape manifold  $R\Sigma_{p,0}^k$  is the set of size-and-reflection-shapes in general position of size one, submanifold of  $SR\Sigma_{p,0}^k$ . Recall the embedding in (20), namely,

$$\psi([\xi]_{RS}) = HJ([\xi]_{RS})H^T = H\xi^T \xi H^T. \quad (37)$$

From Proposition 4.1 and with the notation in Theorem 4.3, it follows that  $\phi(SM_{k,p})$  which is also the range of  $\psi$  in (37) is the set  $\tilde{N}_{p,k}$  of  $(k-1) \times (k-1)$  positive semidefinite symmetric matrices of rank  $p$ , and the restriction of  $\phi$  to  $SM_{p,k}$  is an isometry from  $(SM_{p,k}, d_{k,0})$  to  $(\tilde{N}_{p,k}, d_{k-1,0})$  where  $d_{r,0}$  is the restriction of the Euclidean distance on the space of  $r \times r$  symmetric matrices.

**Remark 6.1.** If, for  $\eta = \xi H$ , we set  $\tilde{\sigma}(\eta) = [\xi]_{RS}$ , the embedding  $\psi$  is equivariant with respect to the group actions of  $O(k-1)$  on  $SR\Sigma_{p,0}^k$  and on  $S(k-1, \mathbb{R})$ :

$$\begin{aligned} \alpha(\tilde{\sigma}(\eta), A) &= \tilde{\sigma}(\eta A) \\ \beta(S, A) &= ASA^T. \end{aligned} \quad (38)$$

In this section we will derive the asymptotics for the extrinsic sample mean size-and-reflection-shape for samples from a  $\psi$ -nonfocal distributions  $Q$  on  $SR\Sigma_{p,0}^k$ . For this purpose we will use the general results for extrinsic means on a manifold in Bhattacharya–Patrangenaru [9, Theorem 3.1 and its corollaries]. The tangent space to  $\tilde{N}_{p,k}$  at  $\psi([\xi]_{RS})$  is the range of the differential of  $\psi$  at  $[\xi]_{RS}$ . If we set  $\eta = \xi H^T$ , then  $\text{rank}(\eta) = p$  and  $\psi([\xi]_{RS}) = \eta^T \eta$ , and

$$T_{\psi(\tilde{\sigma}(\eta))}\tilde{N}_{p,k} = T_{\eta^T \eta}\tilde{N}_{p,k} = \{v \in S(k-1, \mathbb{R}) : v = y^T \eta + \eta^T y, y \in \mathcal{M}(k-1, p, \mathbb{R})\}. \quad (39)$$

Since  $\eta \eta^T$  has an inverse, for any  $y \in \mathcal{M}(k-1, p, \mathbb{R})$  we define the symmetric matrix  $S = \frac{1}{2}(\eta^T (\eta \eta^T)^{-1} y + y^T (\eta \eta^T)^{-1} \eta)$  and obtain the following representation of the tangent space in (40):

$$T_{\eta^T \eta}\tilde{N}_{p,k} = \{v \in S(k-1, \mathbb{R}), v = S \eta \eta^T + \eta^T \eta S, S \in S(k-1, \mathbb{R})\}. \quad (40)$$

Given that the equivariance of  $\psi$ , if  $\eta^T \eta = A \Lambda A^T$ , with  $A \in O(k-1)$  and  $\Lambda$  the diagonal matrix with diagonal elements  $\lambda_1, \dots, \lambda_p, 0, \dots, 0$ , then

$$T_{\eta^T \eta}\tilde{N}_{p,k} = A T_{\Lambda} N_{p,k} A^T. \quad (41)$$

From (40) it follows that the tangent space at  $\Lambda$  is given by

$$T_{\Lambda}\tilde{N}_{p,k} = \left\{ v \in S(k-1, \mathbb{R}), v = \begin{pmatrix} V_p & W \\ W^T & \mathbf{0} \end{pmatrix}, V_p \in S(p, \mathbb{R}), W \in \mathcal{M}(k-1-p, p; \mathbb{R}) \right\}. \quad (42)$$

A standard orthonormal basis in  $S(k-1, \mathbb{R})$  given in [6] is the basis

$$\tilde{E} = (E_1^1, \dots, E_{k-1}^{k-1}, 2^{-\frac{1}{2}}(E_i^j + E_j^i), 1 \leq i < j \leq k-1), \quad (43)$$

where  $E_i^j$  has all entries zero, except that for the entry in the  $i$ th row and  $j$ th column, which equals 1. From (42) it follows that  $T_{\Lambda}\tilde{N}_{p,k}$  is spanned by the orthobasis

$$e(\Lambda) = (E_1^1, \dots, E_p^p, 2^{-\frac{1}{2}}(E_i^j + E_j^i), 1 \leq i < j \leq p \text{ or } 1 \leq i \leq p < j \leq k-1). \quad (44)$$



Since, for any  $A \in O(k-1)$ , the map  $v \rightarrow AvA^T$  is an isometry of  $S(k-1, \mathbb{R})$ , an orthobasis in the space  $T_{\eta^T \eta} \tilde{N}_{p,k}$  is then given by

$$e(\eta^T \eta) = (E_1^1(\eta), \dots, E_p^p(\eta), 2^{-\frac{1}{2}}(E_i^j(\eta) + E_j^i(\eta))), \quad 1 \leq i < j \leq p \text{ or } 1 \leq i \leq p < j \leq k-1, \quad (45)$$

where  $E_i^j(\eta) = AE_i^jA^T$ .

**Remark 6.2.** Since the asymptotic results are often presented in vector notation, it will be useful to order the orthobasis (43) in the following noncanonical way

$$E = (E_1^1, \dots, E_p^p, 2^{-\frac{1}{2}}(E_i^j + E_j^i), 1 \leq i < j \leq p \text{ or } 1 \leq i \leq p < j \leq k-1, \\ E_{p+1}^{p+1}, \dots, E_{k-1}^{k-1}, 2^{-\frac{1}{2}}(E_i^j + E_j^i), p+1 \leq i < j \leq k-1). \quad (46)$$

From Section 5, the extrinsic mean  $\mu_E = \mu_{\psi, E}(Q)$  of a Schoenberg nonfocal probability measure  $Q$  on  $SR\Sigma_{p,0}^k$  is given by  $\mu_E = \psi^{-1}(P_\psi(\mu))$ , where  $\mu$  is the mean of  $\psi(Q)$  in  $S(k-1, \mathbb{R})$  and  $P_\psi$  is the projection on  $\tilde{N}_{p,k}$ . Following Bhattacharya and Patrangenaru [7], the extrinsic covariance operator  $\Sigma_E = \Sigma_{\psi, E}$  is the restriction of the self-adjoint linear operator  $d_\mu P_\psi \Sigma d_\mu P_\psi^T$  to  $T_{P_\psi(\mu)} \tilde{N}_{p,k}$ . The extrinsic covariance matrix is the matrix associated to  $\Sigma_E$  with respect to an orthobasis  $e_1(P_\psi(\mu)), \dots, e_d(P_\psi(\mu))$  of  $T_{P_\psi(\mu)} \tilde{N}_{p,k}$ ,  $d = \frac{p}{2}(2k-p-1)$ .

**Lemma 6.1.** Assume that the mean  $\mu$  of  $\psi(Q)$  is a diagonal matrix  $\Lambda$ . The differential of the projection  $P_\psi$  at  $\Lambda$  with respect to the ordered orthobasis (46) is given by

$$d_\Lambda P_\psi(E_i^j) = \begin{cases} E_i^j & i \leq p \\ 0 & i > p \end{cases}, \quad d_\Lambda P_\psi(E_j^l + E_l^j) = \begin{cases} E_j^l + E_l^j & j < l \leq p \\ \frac{\lambda_j}{\lambda_j - \lambda_l}(E_j^l + E_l^j) & j \leq p < l \\ 0 & p < j < l. \end{cases} \quad (47)$$

Given that the equivariance of the embedding  $\psi$ , from Lemma 6.1 we obtain the following

**Proposition 6.1.** If the spectral decomposition of the mean  $\mu$  of  $\psi(Q)$  is  $\mu = \sum_{i=1}^{k-1} \lambda_i \tilde{e}_i \tilde{e}_i^T$ , with  $\lambda_1 \geq \dots \geq \lambda_p > \lambda_{p+1} \geq \dots \geq \lambda_{k-1}$ , then

(i) the tangent space  $T_{\psi(\mu_E)} N_{p,k} = T_1 \oplus T_2$ , where  $T_1$  has the orthobasis

$$(\tilde{e}_1 \tilde{e}_1^T, \dots, \tilde{e}_p \tilde{e}_p^T, 2^{-\frac{1}{2}}(\tilde{e}_i \tilde{e}_j^T + \tilde{e}_j \tilde{e}_i^T), (1 \leq i < j \leq p)), \quad (48)$$

and  $T_2$  has the orthobasis

$$(2^{-\frac{1}{2}}(\tilde{e}_j \tilde{e}_l^T + \tilde{e}_l \tilde{e}_j^T), 1 \leq j \leq p < l \leq k-1). \quad (49)$$

(ii) Let  $N$  be the orthocomplement of  $T_{\psi(\mu_E)} N_{p,k}$ . Then if

$$d_\mu P_\psi|_{T_1} = Id_{T_1}, \\ d_\mu P_\psi(\tilde{e}_j \tilde{e}_l^T + \tilde{e}_l \tilde{e}_j^T) = \frac{\lambda_j}{\lambda_j - \lambda_l}(\tilde{e}_j \tilde{e}_l^T + \tilde{e}_l \tilde{e}_j^T), \quad \forall(j, l), 1 \leq j \leq p < l \leq k-1, \\ d_\mu P_\psi|_N = 0. \quad (50)$$

An orthobasis of  $N$  in Proposition 6.1 is

$$2^{-\frac{1}{2}}(\tilde{e}_j \tilde{e}_l^T + \tilde{e}_l \tilde{e}_j^T), \quad (p < j < l \leq k-1). \quad (51)$$

The two orthobases (48), (49) and (51) yield an orthobasis  $\tilde{\mathbf{e}}$  of  $S(k-1, \mathbb{R})$ . From Proposition 6.1 it follows that the matrix  $D$  associated with the differential  $d_\mu P_\psi$  relative to the orthobasis  $\tilde{\mathbf{e}}$  is diagonal:

$$D = \begin{pmatrix} I_{\frac{p(p-1)}{2}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Delta_{p(k-p-1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad (52)$$

where

$$\Delta_{p(k-p-1)} = \begin{pmatrix} \frac{\lambda_1}{\lambda_1 - \lambda_{p+1}} & \cdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \cdots & \frac{\lambda_p}{\lambda_p - \lambda_{k-1}} \end{pmatrix}. \quad (53)$$

The space of symmetric matrices  $S(k-1, \mathbb{R})$  regarded as its own tangent space at  $\mu$  splits into three orthogonal subspaces

$$S(k-1, \mathbb{R}) = T_1 \oplus T_2 \oplus N, \quad (54)$$

leading to a decomposition of the covariance matrix  $\Sigma$  of  $\psi(Q)$ , with respect to the orthobasis of  $S(k-1, \mathbb{R})$  obtained by augmenting the orthobasis (44) by an orthobasis of  $N$ , as follows:

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{12}^T & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{13}^T & \Sigma_{23}^T & \Sigma_{33} \end{pmatrix}. \quad (55)$$

If we change the coordinates in  $\mathbb{R}^{k-1}$  by selecting an orthobasis  $\tilde{\mathbf{e}}$ , the eigenvectors  $\tilde{e}_1, \dots, \tilde{e}_{k-1}$  of  $\mu$ , in such a coordinate system, the mean is a diagonal matrix  $\Lambda$  and the matrix  $\Sigma_\mu = D\Sigma D^T$ , defined in [7] is

$$\Sigma_\mu = \begin{pmatrix} \Sigma_{11} & \Sigma_{12}\Delta & 0 \\ \Delta\Sigma_{12}^T & \Delta\Sigma_{22}\Delta & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (56)$$

and the extrinsic covariance matrix  $\Sigma_E$  defined in [7], with respect to the basis  $d_{\mu_\psi}^{-1}(e(\Lambda))$ , with  $e(\Lambda)$  as defined in (44), is

$$\Sigma_E = \begin{pmatrix} \Sigma_{11} & \Sigma_{12}\Delta \\ \Delta\Sigma_{12}^T & \Delta\Sigma_{22}\Delta \end{pmatrix}. \quad (57)$$

We assume now that  $Y_1, \dots, Y_n$  are independent identically distributed random reflection objects from a  $\psi$ -nonfocal probability distribution  $Q$  on  $S\Sigma_{p,0}^k$ , with  $\lambda_p > \lambda_{p+1}$  and let  $\tilde{s\bar{o}}(\eta)$  be the mean of  $\psi(Q)$  and  $\Sigma$  the covariance matrix of  $\psi(Q)$  with respect to the orthobasis  $\tilde{\mathbf{e}}$  defined above. Let  $\vec{W}$  be the vectorized form of a matrix  $W \in S(k-1, \mathbb{R})$  with respect to the basis  $\tilde{\mathbf{v}}$ . Assume  $\tan \vec{W}$  denote the component of  $\vec{W}$  tangent to  $\tilde{N}_{p,k}$  at  $\vec{\psi}(\mu_\psi)$ .

**Theorem 6.1.** (a) The random vector  $n^{\frac{1}{2}} \tan(\vec{\psi}(\bar{Y}_E) - \vec{\psi}(\mu_E))$  converges weakly to a random vector having an  $N(0, \Sigma_E)$  distribution, where  $\Sigma_E$  is given in (57).

(b) If  $\Sigma_E$  is nonsingular, then  $n \tan(\vec{\psi}(\bar{Y}_E) - \vec{\psi}(\mu_E))^T \Sigma_E^{-1} \tan(\vec{\psi}(\bar{Y}_E) - \vec{\psi}(\mu_E))^T$  converges weakly to a  $\chi_{kp - \frac{p(p+1)}{2}}^2$  distribution.

From Theorem 6.1 we obtain the following result:

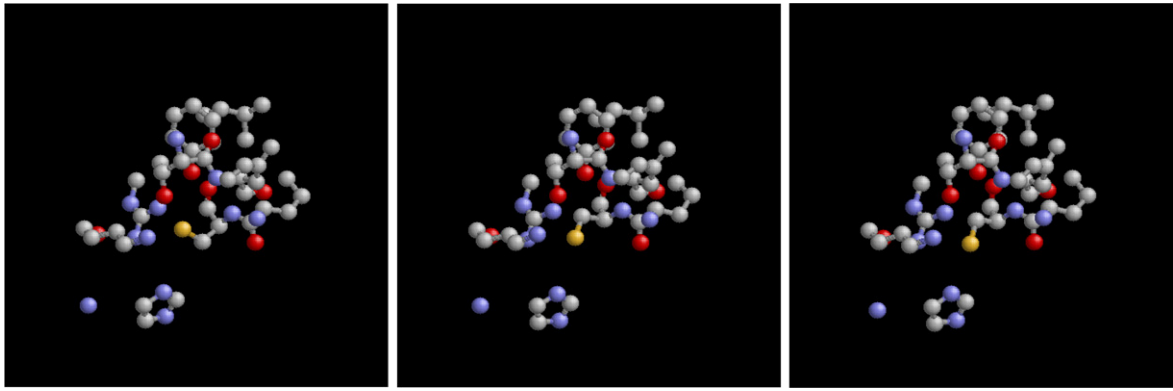
**Corollary 6.1.** Let  $G$  be a normally distributed matrix in  $S(k-1, \mathbb{R})$ , weak limit of  $n^{\frac{1}{2}}(\bar{Y} - \mu)$ . Assume that the spectral decomposition of  $\mu$  is  $\mu = V\Lambda V^T$ . Set  $G^V = V^T G V = (g_{jl}^V)$  and  $\tilde{G}^V = (\tilde{g}_{jl}^V)$  be determined by

$$\tilde{g}_{jl}^V = \begin{cases} g_{jl}^V & 1 \leq j \leq l \leq p \\ \frac{\lambda_j}{\lambda_j - \lambda_l} g_{jl}^V & 1 \leq j \leq p < l \leq p-1 \\ 0 & p < j \leq l \leq k-1. \end{cases} \quad (58)$$

Then  $n^{\frac{1}{2}}(\psi(\bar{Y}_E) - \psi(\mu_E))$  converges in distribution to the normally distributed random matrix  $VG^V V^T$ .

From Theorem 6.1 it follows that the extrinsic mean size-and-reflection-shape can be easily estimated using nonpivotal bootstrap. Assume that  $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  is a random sample of configurations  $\mathbf{x}_j = (x_j^1, \dots, x_j^k)$ ,  $j = 1, \dots, n$ . We resample at random and with repetition  $N$  times from this sample, where  $N$  is a reasonably large number, say  $N \geq 500$ . For each such resample  $\mathbf{x}_1^*, \dots, \mathbf{x}_n^*$  we compute the extrinsic sample mean  $[\mathbf{x}]_{RS_E}^*$ . We then use a local parametrization of  $S\Sigma_{p,0}^k$  and find  $(1 - \alpha)100\%$  Bonferroni simultaneous confidence intervals for the corresponding  $kp - \frac{p(p+1)}{2}$  local coordinates.

**Remark 6.3.** Similarly nonpivotal bootstrap can be used to estimate extrinsic mean reflection shapes. Pivotal bootstrap distributions for extrinsic sample means size-and-reflection-shapes and resulting confidence regions for extrinsic sample Schoenberg means, will be presented in another paper.



**Fig. 1.** Protein structures. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Two sample tests for extrinsic means on manifolds can be derived from the general theory for two sample tests for extrinsic means on manifolds recently developed by Bhattacharya [11].

**Remark 6.4.** For extrinsic mean size-and-reflection-shapes,  $k = p + 1$ , from Remark 4.1, it follows that the space  $SR\Sigma_{p,0}^{p+1}$  is isometric to a convex open subset of a Euclidean space of dimension  $\frac{p(p+1)}{2}$  and, in view of Remark 5.1 this isometry carries the extrinsic means to ordinary means in this Euclidean space, and inference for means on  $SR\Sigma_{p,0}^{p+1}$  follows from multivariate analysis. In particular, for  $k = p + 1$ , at level  $\alpha$ , a nonpivotal bootstrap test for the matched paired hypothesis  $H_0 : \mu_{1,E} = \mu_{2,E}$  can be obtained as follows. Given that matched pair samples  $[\mathbf{x}_{1,i}]_{RS}, [\mathbf{x}_{2,i}]_{RS}, i = 1, \dots, n$ , consider  $100(1-\alpha)$  simultaneous confidence intervals for the mean difference matrix  $\psi(\mu_{1,E}) - \psi(\mu_{2,E})$  obtained from the bootstrap distribution of  $\overline{\psi([\mathbf{x}_1]_{RS})} - \overline{\psi([\mathbf{x}_2]_{RS})}$ , and reject  $H_0$  if at least one of these intervals does not contain 0.

## 7. Applications to medical imaging

In medical imaging, or in bioinformatics shape analysis or shape-and-size based classification is often used to identify mean differences between two populations of planar or volumetric images of the same type of anatomical scenes. Shape changes due to a disease, or caused by aging, as size or volume changes have been widely used. Here we give one example of application of our results in Section 4, and two examples of applications of our results in Sections 5 and 6 to landmark based size-and-reflection-shape difference in medical imaging.

### 7.1. Mean protein structures

This example graphically illustrates the computation of the extrinsic sample mean size-and-reflection-shape, based on a sample of size 3. For more computational examples see Su et al. [16]. Here  $k = 63$ , so that the dimension of the three-dimensional size-and-reflection-shape-manifold is  $d = 183$ . The extrinsic sample mean is therefore represented in Fig. 2. For the coordinates of atoms in the matched configurations we refer to the Protein Data Bank (PDB). PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease. We consider here three examples of *phosphotransferase/inhibitors*, obtained by X-ray diffraction (the size is measured in Å). Their structures id's on PDB are 1ydr, 1yds and 1ydt. Images of matched configurations of atom coordinates for these proteins from PDB are obtained in RasMol form of original macromolecules. The PDB Primary Citation for these proteins is Engh et al. [17]. In Fig. 1 we display the matched color coded configurations of more than 50 atoms (red = hydrogen, blue = oxygen, gray = carbon, yellow = sulphur) and in Fig. 2, their extrinsic sample size-and-reflection-shape mean.

### 7.2. Application to glaucoma detection

Glaucoma is the third leading cause of loss of vision. It is responsible worldwide for tens of millions of cases of blindness. For more statistics on glaucoma see Epstein et al. [18]. This subsection is devoted to a study of glaucomatous size-and-reflection-shape change detection using three-dimensional data analysis. We consider a set of three-dimensional laser range data from the LSU Experimental Glaucoma Study. The Optic Nerve Head (ONH) of both eyes of 12 mature rhesus monkeys were imaged on three separate sessions with a Scanning Confocal Laser Tomograph (SCLT). One of the eyes was treated to increase the Intra Ocular Pressure (IOP) which is often the case of the glaucoma onset. To find out more about the LEGS study and the image acquisition, see Burgoyne et al. [19]. For details on landmark registration see Derado et al. [20]. The

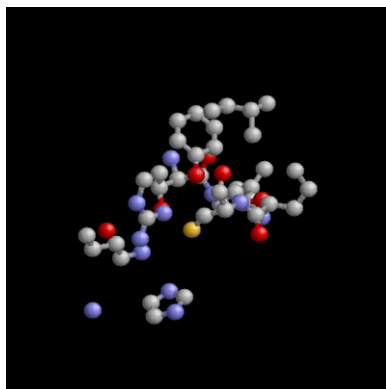


Fig. 2. Extrinsic sample mean reflection-size-and-shapes of matched configurations protein structures in Fig. 1.

landmark coordinates can be found in Bhattacharya and Patrangenaru [7]. Note that the images were taken all from the same distances and angles, so that the sizes are consistent throughout the resulting image data library. The four landmarks in the ONH region are S for the superior aspect of the retina toward the top of the head, N for the nasal or nose side of the retina, T for temporal, the side of the retinal closest to the temple or temporal bone of the skull and V for the ONH deepest point. These four landmarks and their positions on the papilla and the deepest point of the ONH cup are schematically displayed in Fig. 3 below from (see [7]). Note that while in the previous analyses of this data sets the landmarks N and T have been considered the same both in the healthy and in the diseased eye, this is not always the case, since due to the facial symmetry they are the same up to a reflection. Our analysis in this section avoids this potential problem, since in similarity shape analysis, configurations are also identified up to a mirror symmetry. In this paper we will test for mean glaucomatous size-and-reflection-shape change (a test for the reflection-shape change was run by Bhattacharya [11]). For the present matched data, a difference in size, as well as in shape, between the normal and the glaucomatous eyes of a monkey should be considered a more appropriate diagnostic feature than the difference in shape alone. Hence statistical testing of mean difference is important for such matched pair of observations. From Remark 6.4, we carry out an analysis for the equality of means on the convex set of symmetric matrices  $S_+(3, \mathbb{R})$ . To each size-and-reflection-shape data point  $[\mathbf{x}]_{RS}$ , we associate the matrix  $\psi([\mathbf{x}]_{RS}) \in S_+(3, \mathbb{R})$ , using Eq. (20). Our choice for the matrix  $H$  there is

$$H = \frac{1}{2} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \quad (59)$$

The six coordinates on the size-and-reflection-shape manifold  $SR\Sigma_{3,0}^4$  are the entries of the upper triangular submatrix of a symmetric matrix:  $(b_{11}, b_{12}, b_{13}, b_{22}, b_{23}, b_{33})$ . For the bootstrap confidence region we used 1000 resamples, for the differences between the local similarity shape coordinates of the paired glaucomatous vs control eye. A 95% bootstrap c. r. in the difference between these size-and-reflection-shape coordinates divided by  $10^5$  given below

L	−1.0478	−1.5055	−0.5826	−1.9424	−0.1169	−0.0436
U	+0.5216	−0.1141	+0.3014	−0.0584	+0.2693	+1.3689

shows that the extrinsic means are significantly different in the treated vs glaucomatous eye at a 5% level of significance. The individual c.i. for each marginal is at level 0.992.

### 7.3. Application to X-Ray cranial differences in children

Consider now the problem of testing if two population mean planar shapes (respectively planar size-and-shapes) are the same. Recently analytical computations of such nonparametric tests using the explicit Jacobian of the embedding, which can be implemented numerically with some effort, have been obtained for distributions on the Kendall two-dimensional shape spaces by Bhattacharya and Bhattacharya [21]. But coverage errors of such asymptotic tests may be considerable for the high-dimensional shape spaces, when based on relatively small sample sizes that are generally available. Therefore we have resorted to bootstrapping. However, as is well known, bootstrapping of tests are generally based on first bootstrapping confidence regions and then using duality. Unlike the large sample estimation of the difference of two multivariate means of distributions on a Euclidean space by an elliptic confidence region centered at the difference between the two sample means, one cannot subtract one mean shape from another. Also, the tangent spaces at two different points (such as the two mean shapes) on a manifold are completely different objects. While an asymptotic theory of testing for equality may be based on the tangent projections of the two sample shape means on the tangent space at the assumed common population mean, estimating the “difference” between two mean shapes makes no sense in general. We resort to two

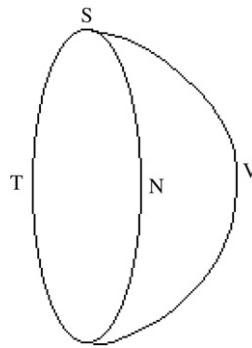


Fig. 3. Four landmarks on the ONH cup relevant in glaucoma.

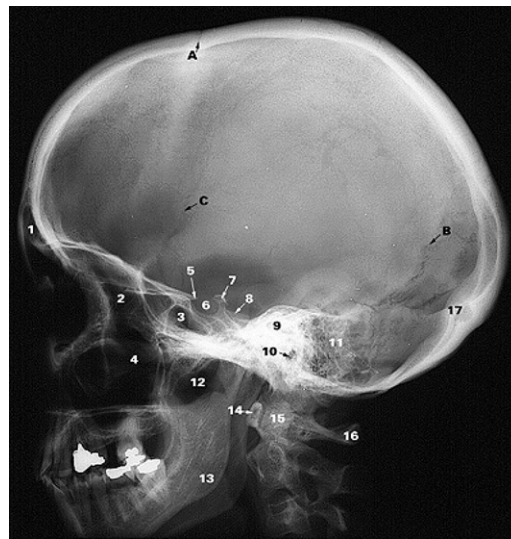


Fig. 4. Landmarks on a lateral X-ray of a child's skull.

strategies: (a) (one-sample) bootstrap confidence regions separately for the two mean shapes, and see if they overlap, and (b) bootstrap a chi-squared like statistic developed in Bhattacharya and Bhattacharya [21] for two sample tests statistic for mean shapes.

**Apert syndrome vs clinically normal children.** As an application of results presented in Section 5, we test if the mean shapes of five common craniofacial landmarks for Apert syndrome children and for healthy children are the same. The Apert data sample is from Bookstein [22, pp. 405–406] and the clinically healthy children sample is from the University School data in the same book, pp. 400–405. There are about 40 anatomical landmarks on the skull listed in Bookstein [22], some of which are displayed in Fig. 4. Out of these only 8 landmarks are registered in the healthy group. An equal number of landmarks is registered in the diseased group. The two groups share only 5 registered landmarks, that are considered here. The shape variable (in our case, shape of the 5 landmarks on the upper mid-face) is valued in  $\Sigma_2^5$  (real dimension = 6).

(a) Nonpivotal bootstrap distributions for the extrinsic mean shape of this configurations are computed using 500 resamples. The 100% confidence regions for the extrinsic means (i.e., the full range of the bootstrapped means) using the three simultaneous bootstrap complex intervals in Bhattacharya and Patrangenaru (2005) [7] are as follows.

For the Apert Kids: for  $w_1$ :

$$(0.7111 - 1.3084i, 0.4316 - 1.2964i),$$

for  $w_2$ :

$$(-1.3280 + 0.4314i, -1.2228 + 0.3610i),$$

and for  $w_3$ :

$$(-0.3548 - 0.4551i, -0.2826 - 0.2870i).$$

For the normal Kids: for  $w_1$ :

$$(0.1766 - 1.2780i, 0.3061 - 1.1140i),$$

for  $w_2$ :

$$(-1.1739, 0.5124i, -1.1096 + 0.3855i),$$

and for  $w_3$ :

$$(-0.3149 - 0.6500i, -0.2630 - 0.5558i).$$

Note that the real parts of the second row for the two groups are not overlapping, showing that the extrinsic mean shapes of the Apert group, and of the normal population are different at every level of significance, however small. If we use the procedure (b) to compare the mean shapes, the test statistic in Bhattacharya and Bhattacharya [21] has the  $P$ -value  $p = 1.4362e-004$ , also showing a highly significant difference between the two groups.

**Remark 7.1.** A comparison to a more conventional Procrustes type analysis is left as an exercise to the reader specialized in classical shape analysis.

**Size-and-shape in clinically normal children.** Referring to the University School data in the example above, we divided the data sets into two equal size groups of large respectively small size, and then tested for the equality of extrinsic means of shapes in this groups. The  $P$ -values for testing the equality of extrinsic mean shapes for small vs big sizes are 0.0123 in the male population and 0.0265 in the female population, showing significant mean shape difference between groups of different sizes. We, therefore, compute extrinsic mean shape in the small size group vs the large size group separately for males and females:

- in the male population:

$$[\bar{\mathbf{x}}]_{E, \text{small}} = [(-0.0607 + 0.3107i, -0.4349 - 0.0296i, 0.2328 + 0.2635i, 0.3443 + 0.0042i, 0.2326 - 0.4640i, -0.1964 + 0.1944i, -0.1816 - 0.2793i, 0.0639)^T]$$

$$[\bar{\mathbf{x}}]_{E, \text{large}} = [(-0.0887 + 0.3006i, -0.4312 - 0.0451i, 0.2127 + 0.2684i, 0.3506 + 0.0251i, 0.2748 - 0.4463i, -0.2109 + 0.1870i, -0.1618 - 0.2897i, 0.0545)^T]$$

- in the female population:

$$[\bar{\mathbf{x}}]_{E, \text{small}} = [(-0.0528 + 0.3065i, -0.4347 - 0.0133i, 0.2475 + 0.2517i, 0.3406 + 0.0024i, 0.2223 - 0.4683i, -0.2049 + 0.2002i, -0.1836 - 0.2793i, 0.0656)^T]$$

$$[\bar{\mathbf{x}}]_{E, \text{large}} = [(-0.0554 + 0.3080i, -0.4316 - 0.0138i, 0.2445 + 0.2634i, 0.3438 - 0.0027i, 0.2162 - 0.4758i, -0.1895 + 0.1969i, -0.1846 - 0.2760i, 0.0567)^T].$$

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We thank one of the referees for pointing to [23] and [24] as related references, involving the study of symmetry in planar shape analysis.

## Appendix

The proof of Lemma 6.1 is straightforward. Here we derive only the nontrivial value of the differential on a matrix of the basis (43) in the orthocomplement of the tangent space to  $\psi(\mu_E) = P_\psi(\Lambda)$ . Assume  $\Lambda = \sum_{i=1}^{k-1} \lambda_i E_i = \sum_{i=1}^{k-1} \lambda_i e_i e_i^T$ , and  $j \leq p < l$ . Then

$$(d_\Lambda P_\psi)(E_j^l + E_l^j) = \frac{d}{dt} \Big|_{t=0} \left( t \rightarrow P_\psi \left( \sum_{i=1}^{k-1} \lambda_i e_i + t(e_j e_l^T + e_l e_j^T) \right) \right). \quad (60)$$

Since  $e_1, \dots, e_{j-1}, e_{j+1}, \dots, e_{l-1}, e_{l+1}, \dots, e_{k-1}$  are eigenvectors of  $S(t) = \sum_{i=1}^{k-1} \gamma_i e_i + t(e_j e_l^T + e_l e_j^T)$ , the space spanned by  $e_j, e_l$  is left invariant by  $S(t)$ . Let

$$\lambda_j(t) = \frac{1}{2} \left( \lambda_j + \lambda_l + \sqrt{(\lambda_j - \lambda_l)^2 + 4t^2} \right), \quad \lambda_l(t) = \frac{1}{2} \left( \lambda_j + \lambda_l - \sqrt{(\lambda_j - \lambda_l)^2 + 4t^2} \right) \quad (61)$$



be the eigenvalues of  $S(t)$  and  $e_j(t)$ ,  $e_l(t)$  be the corresponding unit eigenvectors in  $\mathbb{R}e_j \oplus \mathbb{R}e_l$ . Assume for simplicity, the eigenvalue  $\lambda_j$  is a simple. Then for  $|t|$  small enough, the first  $p$  eigenvalues of  $S(t)$  in their descending order are  $\lambda_1 \geq \dots \geq \lambda_{j-1} > \lambda_j(t) > \lambda_{j+1} \dots \geq \lambda_p$  and from Theorem 5.1 it follows that

$$P_\psi(S(t)) = \lambda_j(t)e_j(t)e_j(t)^T + \sum_{i=1, i \neq j}^p \lambda_i e_i e_i^T \quad (62)$$

and

$$\left. \frac{d}{dt} \right|_{t=0} (P_\psi(S(t))) = \left. \frac{d}{dt} \right|_{t=0} (\lambda_j(t)e_j(t)e_j(t)^T) = \lambda_j \left. \frac{d}{dt} \right|_{t=0} (e_j(t)e_j(t)^T), \quad (63)$$

since  $\lambda_j(0) = \lambda_j$ ,  $\lambda_j'(0) = 0$ . The eigenvector  $e_j(t)$  has, up to a sign, the following expression:

$$e_j(t) = \frac{\sqrt{\sqrt{4t^2 + (\lambda_j - \lambda_l)^2} + \lambda_j - \lambda_l}}{2t\sqrt{2\sqrt{4t^2 + (\lambda_j - \lambda_l)^2}}} \left( 2te_j + \left( \sqrt{4t^2 + (\lambda_j - \lambda_l)^2} - (\lambda_j - \lambda_l) \right) e_l \right). \quad (64)$$

Then

$$\begin{aligned} e_j(t)e_j(t)^T &= \frac{\sqrt{4t^2 + (\lambda_j - \lambda_l)^2} + \lambda_j - \lambda_l}{8t^2\sqrt{4t^2 + (\lambda_j - \lambda_l)^2}} \times \left( 4t^2 e_j e_j^T + \left( \sqrt{4t^2 + (\lambda_j - \lambda_l)^2} - (\lambda_j - \lambda_l) \right)^2 e_l e_l^T \right. \\ &\quad \left. + 2t \left( \sqrt{4t^2 + (\lambda_j - \lambda_l)^2} - (\lambda_j - \lambda_l) \right) (e_j e_l^T + e_l e_j^T) \right), \end{aligned} \quad (65)$$

and from (65), it follows that

$$\begin{aligned} e_j(t)e_j(t)^T &= \frac{1}{2} \left( 1 + \frac{\lambda_j - \lambda_l}{\sqrt{4t^2 + (\lambda_j - \lambda_l)^2}} \right) e_j e_j^T + \frac{1}{2} \left( 1 - \frac{\lambda_j - \lambda_l}{\sqrt{4t^2 + (\lambda_j - \lambda_l)^2}} \right) e_l e_l^T \\ &\quad + \frac{t}{\sqrt{4t^2 + (\lambda_j - \lambda_l)^2}} (e_j e_l^T + e_l e_j^T). \end{aligned} \quad (66)$$

Since the derivative of the coefficients of  $e_j e_j^T$ ,  $e_l e_l^T$  respectively, vanishes at  $t = 0$  it turns out that

$$\left. \frac{d}{dt} \right|_{t=0} (e_j(t)e_j(t)^T) = \frac{1}{\lambda_j - \lambda_l} (e_j e_l^T + e_l e_j^T), \quad (67)$$

and from (63) and (67) we obtain

$$d_\Lambda P_\psi(e_j e_l^T + e_l e_j^T) = \frac{\lambda_j}{\lambda_j - \lambda_l} (e_j e_l^T + e_l e_j^T). \quad (68)$$

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