Nonparametric Inference on Shape Spaces

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Abstract. In this talk, I present certain recent methodologies and some new results for the statistical analysis of probability distributions on landmark based shape spaces. The statistical analysis of shape distributions is important in many areas such as morphometrics, medical diagnostics and machine vision. To measure the shape of an object, one may pick a suitable ordered set of k points or landmarks called k-ad or configuration of k points on a two or three dimensional image of the object under consideration. Depending on the way the data are collected or recorded, the appropriate shape of the corresponding k-ad is the maximal invariant specified by the space of orbits under a group of transformations. For example, the equivalence class of the k-ad identified modulo size and Euclidean motions of translation and rotation is called its similarity shape. The shape space can be given a metric tensor and hence a geodesic distance making it a Riemannian manifold. Thus statistical analysis tools developed on general manifolds can be applied to estimate shape parameters and compare different shape distributions. Towards the end, I illustrate that with two examples. This presentation is part of my PhD thesis under Professor Rabi Bhattacharya.

1. Shapes of k-ads

Consider a set of k points or landmarks picked from an object or image in 2D or 3D usually with expert help for purposes of identification, discrimination or diagnostics. Such a set is called a **k-ad** or configuration of k points. In general, each observation $x = (x_1, \ldots, x_k)$ consists of $k > m$ points in m-dimensions (not all same). Depending on the application, the shape of a k-ad is its orbit under a group of transformations and the corresponding shape space consists of all possible orbits. Hence a landmark based shape space M is the quotient of a Riemannian manifold N. For M to be a manifold, we require the action of the group to be free. Then M inherits the Riemannian metric of N and has the natural structure of a Riemannian manifold.

To carry out nonparametric inference on shapes, one may define parameters like mean shape and variation in shape and use their sample estimates to identify a probability distribution. To define such parameters, we choose a suitable distance on M. In my presentation, I propose two such distances which lead to two different approaches for inference on general manifolds, and in particular for landmark based

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shape spaces, namely intrinsic and extrinsic analyses. The **intrinsic analysis** proposed for these spaces is based on their Riemannian structure. Often it is simpler both mathematically and computationally to carry out an **extrinsic analysis** by embedding M into some higher dimensional Euclidean space $E^D(\approx \mathbb{R}^D)$, with the distance induced from that of E^D. This is also pursued when an appropriate Riemannian structure on M is not in sight. Among the possible embeddings, one seeks out **equivariant embeddings** which preserve many of the geometric features of M. In the subsequent sections, I briefly outline the geometry of the different shape spaces that arise in various applications.

1.1. Similarity Shape Spaces Σ_m^k. The **similarity** shape of a k-ad x is its orbit under translations, one dimensional scaling and rotations. To remove the effects of translation and scaling, we bring the center of x to the origin and scale it to have norm 1. Then we get the **preshape** of x which has the expression

$$z = (x_1 - \bar{x}, x_2 - \bar{x}, \ldots, x_k - \bar{x})/\|x - \bar{x}\|$$

where

$$\bar{x} = \frac{1}{k}\sum_{j=1}^{k} x_j,\ \|A\|^2 = \sum_{i=1}^{m}\sum_{j=1}^{k} a_{ij}^2 = \mathrm{Trace}(AA').$$

The set of all preshapes is called the **preshape sphere** and denoted by S_m^k ($\equiv S^{km-m-1}$). The similarity shape of x or of its preshape z is its orbit under all m-dimensional rotations, that is

$$\sigma(x) = \sigma(z) = \{Az\colon A \in SO(m)\}$$

where $SO(m)$ is the special orthogonal group of $m \times m$ orthogonal matrices with determinant $+1$. Hence similarity shape spaces are quotients of the unit sphere S_m^k under the action of $SO(m)$. The action of $SO(m)$ is free when $\mathrm{rank}(z) \geq m-1$. The **similarity shape space** Σ_m^k consists of the shape of all such z, i.e.,

$$\Sigma_m^k = \{\sigma(z) : z \in S_m^k, \mathrm{rank}(z) \geq m-1\}$$

which is a Riemannian manifold of dimension $km - m - \frac{m(m-1)}{2}$.

1.2. Reflection (Similarity) Shape Spaces $R\Sigma_m^k$. Consider now the **reflection shape** of a k-ad as defined in Section 1.1, but with $SO(m)$ replaced by the larger orthogonal group $O(m)$ of all $m \times m$ orthogonal matrices (with determinants either +1 or -1). The **reflection shape space** $R\Sigma_m^k$ is the space of orbits of the elements u of the preshape sphere whose columns span $\mathbb{R}^m$.

For problems in morphometrics, medical diagnostics etc, similarity shape analysis has many use. Recently, for applications in image analysis and machine vision, other notions of shape such as affine and projective shapes have been found to be more appropriate.

1.3. Affine Shape Spaces $A\Sigma_m^k$. The **affine shape** of a k-ad in $\mathbb{R}^m$ may be defined as the orbit of this k-ad under the group of all affine transformations $x \mapsto F(x) = Ax + b$, where A is an arbitrary $m \times m$ non-singular matrix and b is an arbitrary point in $\mathbb{R}^m$. Among numerous applications include bioinformatics-protein matching, machine vision- to reconstruct a larger image from partial views in a number of aerial images and many more.

1.4. Projective Shape Spaces $P\Sigma_m^k$. In machine vision, if images are taken from a great distance, affine shape analysis is appropriate. Otherwise, **projective shape** is a more appropriate choice. If images are obtained through a central projection, a ray is received as a point on the image plane. Since axes in 3D comprise the **projective space** $\mathbb{R}P^2$, k-ads in this view are valued in $\mathbb{R}P^2$. To have invariance with regard to camera angles, one may first look at the original 3D k-ad and achieve affine invariance by its affine shape and finally take the corresponding equivalence class of axes in $\mathbb{R}P^2$, to define the projective shape of the k-ad respect to projective transformations on $\mathbb{R}P^2$. Potential applications of projective shape analysis arise in robotics, particularly in machine vision for robots to visually recognize a scene, avoid an obstacle, e.t.c.

We will return to these shape spaces again in Section 5. Now we turn to nonparametric inference on general manifolds.

2. Fréchet Analysis on Metric Spaces

Let (M, ρ) be a metric space, ρ being the distance on M. For a probability distribution Q on M, define the **Fréchet function** of Q as

$$F(p) = \int_M \rho^2(p, x) Q(dx),\ p \in M.$$

Definition 2.1. Suppose $F(p) < \infty$ for some $p \in M$. Then the set of all p for which $F(p)$ is the minimum value of F on M is called the **Fréchet mean set** of Q. If this set is a singleton, say $\{\mu_F\}$, then μ_F is called the **Fréchet mean** of Q. The minimum value attained by the Fréchet function (if finite) is called the **Fréchet variation** of Q.

If $X_1, X_2, \ldots, X_n$ are independent and identically distributed (iid) with common distribution Q, and $Q_n \doteq (1/n) \sum_{j=1}^n \delta_{X_j}$ is the corresponding empirical distribution, then the Fréchet mean set and the Fréchet variation of Q_n are called the **sample Fréchet mean set** and the **sample Fréchet variation** respectively. By the **sample Fréchet mean**, we will refer to any measurable selection from the sample Fréchet mean set. Proposition 2.1 below, as proved in Bhattacharya and Patrangenaru (2003) establishes the strong consistency of the sample Fréchet mean as an estimator of the Fréchet mean of Q.

Proposition 2.1. *Assume* (i) *that every closed and bounded subset of M is compact, and* (ii) *F is finite on M. Also assume that Q has a unique Fréchet mean μ_F. Then the sample Fréchet mean μ_{F_n} is a strongly consistent estimator of μ_F.*

Next we state the consistency of the sample Fréchet variation in Proposition 2.2. It is proved in Bhattacharya and Bhattacharya (2008a).

Proposition 2.2. *Under assumptions* (i) *and* (ii) *of Proposition 2.1, the sample Fréchet variation V_n is a strongly consistent estimator of the Fréchet variation V of Q.*

Now we consider the asymptotic distributions of μ_{F_n} and V_n. For Theorem 2.3, we assume M to be a differentiable manifold of dimension d. Let ρ be a distance metrizing the topology of M. For a proof, see Bhattacharya and Patrangenaru (2005) and Bhattacharya and Bhattacharya (2008a).

Theorem 2.3. *Suppose the following assumptions hold:*
(i) *Q has support in a single coordinate patch, (U,ϕ), $\phi : U \longrightarrow \mathbb{R}^d$ smooth. Let $Y_j = \phi(X_j)$, $j = 1,\dots,n$.*
(ii) *The Fréchet mean μ_F of Q is unique.*
(iii) *$\forall x,\ y \mapsto h(x,y) = \rho^2(\phi^{-1}x, \phi^{-1}y)$ is twice continuously differentiable in a neighborhood of $\phi(\mu_F) = \mu$.*
(iv) *$E(\mathrm{D}_r h(Y_1,\mu))^2 < \infty\ \forall r$.*
(v) *$E(\sup_{|u-v|\le\epsilon} |\mathrm{D}_s\mathrm{D}_r h(Y_1,v) - \mathrm{D}_s\mathrm{D}_r h(Y_1,u)|) \to 0$ as $\epsilon \to 0\ \forall\ r,s$.*
(vi) *$\Lambda = E\left(\mathrm{D}_s\mathrm{D}_r h(Y_1,\mu)\right)$ is nonsingular.*
Write $\mu_n = \phi(\mu_{F_n})$. Then under the assumptions (i)-(vii)*,*

$$\sqrt{n}(\mu_n - \mu) \xrightarrow{\mathcal{L}} N(0, \Lambda^{-1}\Sigma(\Lambda^{'})^{-1}).$$

Further if $E(\rho^4(X_1,\mu_F)) < \infty$, one has

$$\sqrt{n}(V_n - V) \xrightarrow{\mathcal{L}} N\left(0, \mathrm{Var}(\rho^2(X_1,\mu_F))\right).$$

Depending on what distance we choose on M, we get different notions of means and variations of probability distributions on M. First we start with **intrinsic analysis** where the distance used is the geodesic distance on M.

3. Intrinsic Analysis on Riemannian Manifolds

Let (M,g) be a d-dimensional connected complete Riemannian manifold, g being the Riemannian metric on M. Let the distance $\rho = d_g$ be the geodesic distance under g. Let Q be a probability distribution on M with finite Fréchet function.The Fréchet mean (set) and variation of Q under the distance d_g are called its **intrinsic mean** (set) and **intrinsic variation** respectively. Given a iid random sample $X_1, X_2, \dots, X_n$ from Q, one defines the **sample intrinsic mean** and the **sample intrinsic variation** analogously.

In this section, we will need to use many technical terms related to Riemannian manifolds. For details on them, see DoCarmo (1992) or Lee (1997). We assume that M has all sectional curvatures bounded above by some $C \ge 0$. Then we define $r_* = \min\{\mathrm{inj}(M), \frac{\pi}{\sqrt{C}}\}$ where $\mathrm{inj}(M)$ is the injectivity radius of M. A result due to Kendall(1990) shows that if Q has support in a geodesic ball of radius $\frac{r_*}{2}$, then it has a unique intrinsic mean μ_I in that ball. Then it follows from Theorem 2.3 that under appropriate assumptions, the coordinates of the sample intrinsic mean are asymptotically Normal. Theorem 3.1 as proved in Bhattacharya and Bhattacharya (2008b) gives sufficient conditions for these assumptions to hold. Here we take the coordiante $\phi = \exp_{\mu_I}^{-1}$- the inverse exponential map into tangent space of M at μ_I.

Theorem 3.1. *Assume that Q has support in a geodesic ball of radius $\frac{r_*}{2}$. Let μ_{nI} be the sample intrinsic mean in that ball and let $\mu_n = \phi(\mu_{nI})$. If $\mathrm{supp}(Q) \subseteq B(\mu_I, \frac{r_*}{2})$, then*

$$\sqrt{n}\mu_n \xrightarrow{\mathcal{L}} N(0, \Lambda^{-1}\Sigma\Lambda^{-1}),$$

the parameters Λ and Σ being defined in Theorem 2.3.

To avoid the support restriction, we embed the manifold M into some higher dimensional Euclidean space and carry out an **extrinsic analysis**. Then analysis becomes lot simpler both theoretically and numerically (see Bhattacharya and Patrangenaru (2003,2005), Bhattacharya and Bhattacharya (2008a,b,c)).

4. Extrinsic Analysis on Differentiable Manifolds

Let $J : M \to \mathbb{R}^D$ be an embedding of M into $\mathbb{R}^D$, and let $\tilde{M} = J(M) \subset \mathbb{R}^D$. Define the **extrinsic distance** on M as: $\rho_E(x, y) = \|J(x) - J(y)\|$, where $\|.\|$ denotes Euclidean norm. Let Q have finite Fréchet function

$$F(x) = \int_M \rho_E^2(x, y) Q(dy).$$

The Fréchet mean (set) and variation of Q are called the **extrinsic mean (set)** and **extrinsic variation** of Q respectively. The sample Fréchet mean and variation from an iid random sample $X_1, \dots, X_n$ are called the **sample extrinsic mean** and **sample extrinsic variation** respectively.

In this section, we assume that $\tilde{M}$ is a closed subset of $\mathbb{R}^D$. Then for every $u \in \mathbb{R}^D$ there exists a compact set of points in $\tilde{M}$ whose distance from u is the smallest among all points in $\tilde{M}$. We will call this set **the projection set** of u on $\tilde{M}$ and denote it by $P(u)$. If $P(u)$ is a singleton, u is said to be a **nonfocal point** of $\mathbb{R}^D$ (with respect to $\tilde{M}$); otherwise it is said to be a **focal point** of $\mathbb{R}^D$. Let $Q^J = Q \circ J^{-1}$ be the image of Q in $\mathbb{R}^D$ under J and let $\mu^J = \int_{\mathbb{R}^D} u Q^J(du)$ be the mean of Q^J. Then it is shown in Bhattacharya and Patrangenaru (2003) that the extrinsic mean set of Q is given by $J^{-1}(P(\mu^J))$. Hence Q has a unique extrinsic mean μ_E iff μ^J is a nonfocal point of $\mathbb{R}^D$.

For example on the unit sphere $\mathbb{S}^d$, J is the inclusion map into $\mathbb{R}^{d+1}$ and ρ_E is the chord distance. Any point $u \in \mathbb{R}^{d+1}$ is nonfocal iff $u \neq 0$.

Now we turn to the asymptotic distribution of the sample extrinsic mean μ_{nE} and the sample extrinsic variation V_{nE} when Q has a unique extrinsic mean μ_E. In a neighborhood of a nonfocal point, such as μ^J, the projection map P is smooth and it can be shown that

$$\sqrt{n}(J(\mu_{nE}) - J(\mu_E)) = \sqrt{n} d_{\mu^J} P(\bar{X} - \mu^J) + o_P(1)$$

from which we can derive the asymptotic distribution of μ_{nE} and V_n under fairly mild conditions. This is stated in Theorem 4.1 below. For a proof, see Bhattacharya and Patrangenaru (2005) and Bhattacharya (2008).

THEOREM 4.1. *If Q^J has finite second order moments and μ_E exists, then the (linear) projection of $\sqrt{n}(J(\mu_{nE}) - J(\mu_E))$ on $T_{\mu_E} M$ has asymptotic Normal distribution. Further if Q^J has finite fourth order moments, then $\sqrt{n}(V_{nE} - V_E)$ is asymptotically normal, where V_E is the extrinsic variation of Q.*

One can use Theorems 2.3, 3.1 and 4.1 to construct asymptotic confidence regions for the population means and variations or distinguish between two distributions by comparing the sample means and variations. When the sample sizes are not too large, one may more effectively use Effron's bootstrap methods. For details on such nonparametric tests, see Bhattacharya and Patrangenaru (2003, 2005), Bhattacharya and Bhattacharya (2008a,b,c) and Bhattacharya (2008).

5. Application to Shape Spaces

5.1. Planar Shape Space. Consider the similarity shape space of Section 1.1 in two dimensions. This is called the **planar shape space** or Σ_2^k. For simplicity, a k-ad x is represented by a complex k-vector. Let z be its preshape which lies in the complex sphere $\mathbb{C}S^{k-1} \equiv S^{2k-3}$ ($z \in \mathbb{C}^k$, $\|z\| = 1$, $z'\mathbf{1}_k = 0$). The shape of x is

$$\sigma(x) = \pi(z) = \{e^{i\theta} z : \ -\pi < \theta \leq \pi\}.$$

Then Σ_2^k consists of the shapes of all k-ads x with not all landmarks identical. It is the quotient space S^{2k-3}/S^1 which can be identified with the complex projective space $\mathbb{C}P^{k-2}$. This is a compact Riemannian manifold with all sectional curvatures between 1 and 4 and has an injectivity radius of $\frac{\pi}{2}$. Hence if Q is a probability distribution on Σ_2^k with $\text{supp}(Q) \subseteq B(p, \frac{\pi}{4})$, $p \in M$, then from Section 3 it follows that Q has a unique intrinsic mean.

For extrinsic analysis on Σ_2^k, we embed it into $S(k, \mathbb{C})$, the space of all $k \times k$ complex Hermitian matrices via the **Veronese Whitney** embedding, which is given by

$$J : \Sigma_2^k \to S(k, \mathbb{C}), \ \pi(z) \mapsto zz^* \ (z \in \mathbb{C}S^{k-1}).$$

Let μ^J be the mean of $Q \circ J^{-1}$ viewed as a probability distribution on $S(k, \mathbb{C})$. Then its projection on $J(\Sigma_2^k)$, as defined in Section 4, is given by $P(\mu^J) = \{uu^*\}$, where u is a unit eigen vector corresponding to the largest eigen value of μ^J. The projection is a singleton and Q has a unique extrinsic mean, namely $\pi(u)$, iff the largest eigenvalue of μ^J is simple. This is proved in Bhattacharya and Patrangenaru (2003).

5.2. Reflection Similarity Shape Space $R\Sigma_m^k$. Consider the **reflection similarity shape space** as defined in Section 1.2. For extrinsic analysis on this space, we embed it into $S(k, \mathbb{R})$, the space of all $k \times k$ real symetric matrices via the embedding

$$J : R\Sigma_m^k \to S(k, \mathbb{R}), \ \sigma(x) \mapsto z'z$$

where z is the preshape of the k-ad x. For details on this embedding, see Bandulasiri and Patrangenaru (2005). Given a probability distribution Q, let μ^J be the mean of $Q \circ J^{-1}$ viewed as a probability distribution in $S(k, \mathbb{R})$. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_k$ be eigenvalues of μ^J and let $V_1, V_2, \ldots, V_k$ be the corresponding orthonormal eigenvectors. Let $\bar{\lambda} = \frac{\sum_{j=1}^m \lambda_j}{m}$. Proposition 5.1 below, as proved in Bhattacharya (2008), derives an expression for the projection of μ^J onto $J(R\Sigma_m^k)$ and hence the extrinsic mean set of Q.

PROPOSITION 5.1. *The set of projections of μ^J onto $J(R\Sigma_m^k)$ is given by*

$$P(\mu^J) = \{\sum_{j=1}^m (\lambda_j - \bar{\lambda} + \frac{1}{m}) V_j V_j'\}.$$

It is a singleton and hence Q has a unique extrinsic mean μ_E iff $\lambda_m > \lambda_{m+1}$ and then $\mu_E = \sigma(z)$ where $z = (z_1, \ldots, z_m)'$, $z_j = \sqrt{\lambda_j - \bar{\lambda} + \frac{1}{m}} V_j$.

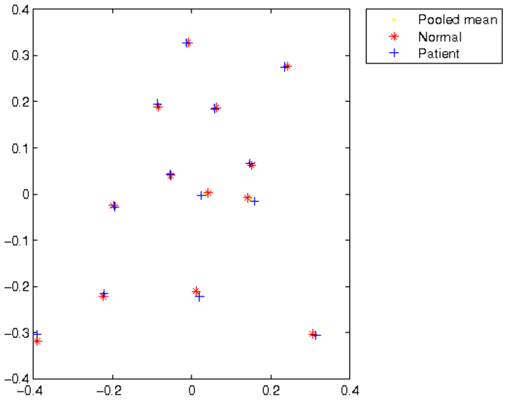

FIGURE 1. Sample extrinsic means' preshapes for the Schizophrenia data

For nonparametric tests to compare the distributions of two random samples on $R\Sigma_m^k$, see Bhattacharya (2008).

6. Applications to Real Data

In this section, we apply the results of shape analysis to two specific applications.

6.1. Schizophrenia Detection. Bookstein (1991) considers 13 landmarks for 14 schizophrenic and 14 normal children on midsagittal 2D slices from MR brain scans. It is of interest to study any shape difference between the brains of the two groups of children, either in mean shape or variation in shape. This is an example of planar shape analysis where we have two independent samples of size 14 each on Σ_2^{13}. In Bhattacharya and Bhattacharya (2008a) asymptotic chi-squared tests are carried out to compare the extrinsic and intrinsic means for the two groups. The corresponding p-values are 3.8×10^{-11} and 3.97×10^{-11} respectively. Also the extrinsic variations are compared by an asymptotic normal test which yields a p-value of 0.3441. Hence we conclude that the mean shapes for the two group of children are different but the variation in shapes are not significantly different. Figure 1 shows the preshapes of the sample extrinsic means along with that of the pooled sample extrinsic mean.

6.2. Glaucoma Detection. Glaucoma is a leading cause of eye blindness. To test if Glaucoma changes the shape of one's eye, 3D images of the Optic Nerve Head (ONH) of both eyes of 12 mature rhesus monkeys were collected. One of the eyes was treated to induce Glaucoma while the other was left normal. 5 landmarks were recorded on each eye. The landmark coordinates can be found in Bhattacharya and Patrangenaru (2005). We consider the reflection shape of the k-ads, so that we have a paired sample of size 12 on $R\Sigma_3^5$. In Bhattacharya (2008), an asymptotic chi-squared test is carried out to compare the mean shapes. The value of the test statistic is 36.56 and the p-value turns out to be 1.38×10^{-5}. Hence we conclude that the mean shapes of the two eyes are significantly different so that Glaucoma

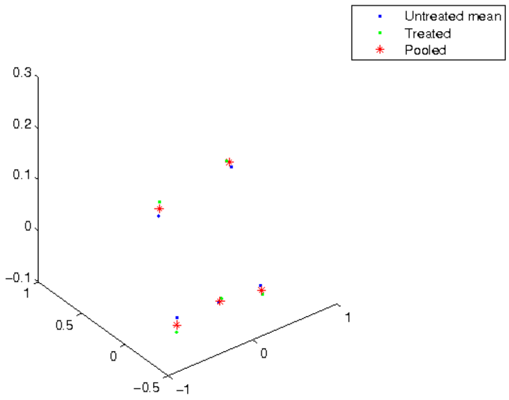

Figure 2. Extrinsic mean shapes for the 2 eyes along with the pooled sample extrinsic mean for the Glaucoma data

indeed changes the shape of the eyes. Figure 2 shows the preshapes of the sample extrinsic means for the two eyes along with the preshape of the pooled sample mean shape.

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