

Nonparametric Inference on Shape Spaces

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Shapes of k-ads

- k points are picked from an object in 2D or 3D usually with expert help called **k-ad** or configuration of k points.
- In general, each observation $\mathbf{x} = (x_1, \dots, x_k)$ consists of $k > m$ points in m -dimension (not all same).
- Shape of a k-ad is its orbit under a group G of transformations.

Kendall's (Direct Similarity) Shape Space Σ_m^k

[Kendall(1984)]

- G is generated by translations, scaling and rotations.
- **Preshape** of a k-ad is

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

where

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

- Set of all preshapes is the **Preshape Sphere**
 $S_m^k \equiv S^{km-m-1}$.

- Similarity shape of x is

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

- Σ_m^k is the set of all such shapes,

$$\Sigma_m^k = S_m^k / SO(m).$$

- $SO(m)$ acts freely when $\text{rank}(z) \geq m - 1$.
- Then Σ_m^k is a Riemannian manifold of dimension $km - m - \frac{m(m-1)}{2}$.

Reflection Shape Space $R\Sigma_m^k$

- $R\Sigma_m^k = S_m^k / O(m)$.
- For $O(m)$ to act freely, assume $\text{rank}(z) = m$.
- Then $R\Sigma_m^k$ is a Riemannian manifold.

Affine Shape Space $A\Sigma_m^k$

- The **affine shape** of a k-ad x in \mathbb{R}^m is its orbit under the group of all affine transformations.
- $A\Sigma_m^k = H_m^k / GL(m)$ where H_m^k consists of all centered k-ads whose landmarks span \mathbb{R}^m and $GL(m)$ is the set of all $m \times m$ nonsingular matrices.
- Can be identified with the **Grassmanian** $G_m(k-1)$: the set of all m dimensional subspaces of \mathbb{R}^{k-1} (Sparr(1995)).
- Manifold of dimension $km - m - m^2$.

Projective Shape Space $P\Sigma_m^k$

- Landmarks of the k-ad viewed in $\mathbb{R}P^m$ -the set of all lines through origin in \mathbb{R}^{m+1} .
- Projective transformation α on $\mathbb{R}P^m$ defined by $A \in GL(m+1)$:

$$\alpha([y]) = [Ay]$$

where $y = (y^1, \dots, y^{m+1})' \in \mathbb{R}^{m+1} \setminus \{0\}$, $[y]$ is the line through y :

$$[y] = \{\lambda y : \lambda \neq 0\}.$$

- $PGL(m)$ is the group of all projective transformations on $\mathbb{R}P^m$.

- For a k-ad $x = (x_1, \dots, x_k)$ in $(\mathbb{R}P^m)^k$, its **projective shape** is its orbit under $PGL(m)$, i.e.,

$$\sigma(x) = \{(\alpha x_1, \dots, \alpha x_k) : \alpha \in PGL(m)\}.$$

- A k-ad x is in **general position** if it has at least $m + 2$ landmarks, the linear span of any $m + 1$ points from which is $\mathbb{R}P^m$.
- The space of projective shapes of all k-ads in general position is $P\Sigma_m^k$.
- Riemannian manifold of dimension $m(k - m - 2)$.

Relation between different notions of shapes of k-ads

- When images/photos obtained through a central projection, like a pinhole camera, projective shape analysis is useful.
- For images taken from a great distance, the rays from the object almost parallel to the camera plane. Then affine shape analysis appropriate.
- Further if the rays are perpendicular to the camera plane, similar shapes can be used.

Fréchet Function of Probability Q on Manifold M

- Let ρ be a distance metrizing the topology of M .
- Assume all closed and bounded subsets are compact.
- For a probability measure Q on M , its **Fréchet function** is defined as

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

Fréchet Mean and Variation of Q on M

Definition

Fréchet mean set of Q is the set of minimizers of the Fréchet function F . A unique minimizer (if exists) is called the **Fréchet mean** of Q , say μ_F .

Definition

The minimum value attained by F (if finite) is called the **Fréchet variation** of Q .

Sample Fréchet Mean and Variation

Definition

Given an iid sample X_1, \dots, X_n from Q , the **sample Fréchet mean** μ_{F_n} is a measurable selection from the Fréchet mean set of the empirical distribution Q_n .

Definition

The Fréchet variation of Q_n is called the **sample Fréchet variation**.

Consistency and Asymptotic Distribution of Sample Fréchet Mean

Proposition

(BP(2003)) If Q has a unique Fréchet mean μ_F , then the sample Fréchet mean μ_{F_n} is a strongly consistent estimator of μ_F .

Theorem

(BP(2005)) If Q has support in a single coordinate patch (U, ϕ) , under appropriate assumptions, $\sqrt{n}(\phi(\mu_{F_n}) - \phi(\mu_F))$ has asymptotically mean 0 Gaussian distribution.

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(BB(2008a)) If F is finite on M , then the sample Fréchet variation V_n is a strongly consistent estimator of the Fréchet variation V of Q .

Theorem

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Intrinsic Mean on Riemannian Manifold (M, g)

- g is the Riemannian metric tensor on M .
- $\rho = d_g$: geodesic distance under g .
- Fréchet mean of probability Q is called the **intrinsic mean** of Q .

Define $r_* = \min\{\text{inj}(M), \frac{\pi}{\sqrt{C}}\}$ where $\text{inj}(M)$ is the injectivity radius of M and $C \geq 0$ is an upper bound on sectional curvatures of M .

Proposition

(Kendall(1990)) 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.*

- Let μ_{nl} be the **sample intrinsic mean** from iid sample $X_1, \dots, X_n \sim Q$.
- Let $\phi = \exp_{\mu_l}^{-1}$: the inverse exponential map into tangent space of M at μ_l . $\mu_n = \phi(\mu_{nl})$.

Theorem

(BB(2008b)) If $\text{supp}(Q) \subseteq B(\mu_l, \frac{r_}{2})$, then $\sqrt{n}\mu_n$ has a nonsingular mean 0 asymptotic Gaussian distribution in $T_{\mu_l}M$.*

Extrinsic Mean of Probab. Q on Manifold M

- Let $J: M \rightarrow \mathbb{R}^D$ be an **embedding equivariant** under some group action H .
- $\rho = \rho_E$ is the distance induced by this embedding. Called the **Extrinsic distance**.

Definition

Let Q have finite Fréchet function

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

The Fréchet mean of Q (if unique) is called the **Extrinsic mean** of Q .

- Let μ^J be the mean of image $Q \circ J^{-1}$ of Q in \mathbb{R}^D .
- Identify M with $J(M)$.
- $P(\mu^J)$ = Set of projections of μ^J on M .

Proposition

(BP(2003)) If $P(\mu^J)$ is singleton, then $\mu_E = P(\mu^J)$ is the extrinsic mean of Q .

- Example.

$$M = S^d = \{p \in \mathbb{R}^{d+1} : p = 1\}.$$

J = Inclusion map, ρ_E = Chord distance,

$$\mu^J = \int_{S^d} xQ(dx) \in \mathbb{R}^{d+1}. \mu_E = \frac{\mu^J}{\|\mu^J\|} \text{ unique iff } \mu^J \neq 0.$$

Sample Extrinsic Mean

- X_1, \dots, X_n iid sample from Q on M (identified with $J(M)$).
- **Sample extrinsic mean** μ_{nE} is a measurable selection from $P(\bar{X})$.

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

Theorem

(BP(2005), Abhishek(2008)) If Q^J has finite 2nd moments and μ_E exists, then the (linear) projection of $\mu_{nE} - \mu_E$ in the tangent space of M at μ_E is asymptotically Gaussian.

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Geometry of Σ_2^k

- k -ad x represented by a complex k -vector ($\in \mathbb{C}^k$).
- Let \mathbf{z} be its preshape. ($\mathbf{z} \in \mathbb{C}^k$, $\|\mathbf{z}\| = 1$, $\mathbf{z}'\mathbf{1}_k = 0$)
- Shape of x is

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

- $\Sigma_2^k \simeq \mathcal{S}^{2k-3}/\mathcal{S}^1 \simeq \mathbb{C}P^{k-2}$.

Intrinsic Mean on Σ_2^k

- Identified with $\mathbb{C}P^{k-2}$, Σ_2^k is compact Riemannian manifold.
- All sectional curvatures between 1 and 4.
- Injectivity radius = $\frac{\pi}{2}$.
- If $\text{supp}(Q) \subseteq B(p, \frac{\pi}{4})$, Q has a unique intrinsic mean.

Extrinsic Mean on Σ_2^k

- Embedding

$$J : \Sigma_2^k \rightarrow S(k, \mathbb{C}) \text{ (} k \times k \text{ Hermitian matrices)}$$
$$\sigma(x) \mapsto \mathbf{z}\mathbf{z}^*$$

- J is H -equivariant, $H = SU(k)$: $k \times k$ matrices A , $AA^* = I_k$, $\det(A) = +1$.

$\mu^J = \text{Mean of } Q \circ J^{-1}$: positive semi definite, rank ≥ 1 , trace = 1, $\mu^J \mathbf{1}_k = 0$.

Proposition

(BP(2003)) μ_E exists iff the largest eigenvalue λ_k of μ^J is simple. Then $\mu_E = [m]$, m unit eigenvector corresponding to λ_k .

Extrinsic Analysis on $R\Sigma_m^k$

- Embedding

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

- J is H -equivariant, $H = O(k)$.
- $J(R\Sigma_m^k) = \{A : A = A', A \text{ is p.s.d.}, \text{Rank}(A) = m, \text{Trace}(A) = 1, A\mathbf{1}_k = \mathbf{0}\}$.
- $J(R\Sigma_m^k)$ submanifold of $S(k, \mathbb{R})$ (not complete).

Extrinsic Mean on $R\Sigma_m^k$

$\mu^J = \text{Mean of } Q \circ J^{-1} \text{ in } S(k, \mathbb{R}): \text{p.s.d. of rank } \geq m, \text{ Trace} = 1,$
 $\mu^J \mathbf{1}_k = 0.$

Proposition

(Abhishek(2008)) Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$ be eigenvalues of μ^J and V_1, V_2, \dots, V_k be corresponding orthonormal eigenvectors.

Let $\bar{\lambda} = \frac{\sum_{j=1}^m \lambda_j}{m}$.

(i) μ_E exists iff $\lambda_m > \lambda_{m+1}$ and then

(ii) $J(\mu_E) = \sum_{j=1}^m (\lambda_j - \bar{\lambda} + \frac{1}{m}) V_j V_j'$, $\mu_E = \sigma(z)$ where

$z = [z_1, \dots, z_m]'$, $z_j = \sqrt{\lambda_j - \bar{\lambda} + \frac{1}{m}} V_j$.

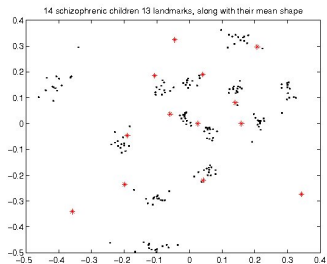
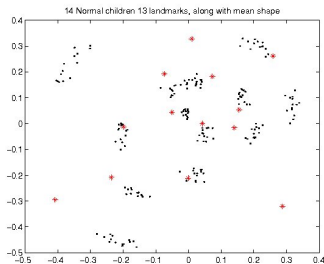
1. Schizophrenic children vs normal children

- 13 landmarks for 14 schizophrenic & 14 normal children on a midsagittal 2D slice from MR brain scan. (Bookstein(1991))
- 2 independent samples of size 14 on Σ_2^k , $k = 13$ (dimension = 22).
- Extrinsic test statistic for comparing the extrinsic mean shapes = 95.5476. (BB(2008a))
- p-value = $P(\chi_{22}^2 > 95.5476) = 3.8 \times 10^{-11}$.

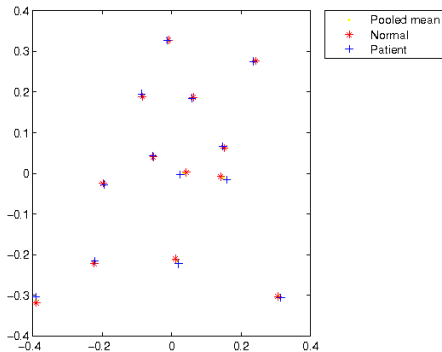
Schizophrenia analysis: mean & variation comparisons

- Intrinsic test statistic = 95.4587, p-value = 3.97×10^{-11} . (BB(2008a))
- Extrinsic sample variations for patient and normal samples are 0.0107 and 0.0093 respectively.
- Test statistic for testing equality of extrinsic variations = 0.9461. (BB(2008a))
- p-value = $P(|Z| > 0.9461) = 0.3441$. ($Z \sim N(0, 1)$.)

Schizophrenia plots: sample k-ads



Schizophrenia plots: Extrinsic mean shapes



2. Glaucoma detection

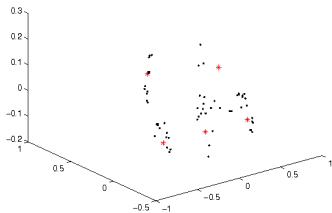
- 5 landmarks on the glaucoma induced eye and the normal eye of 12 rhesus monkeys. (BP(2005))
- Paired samples of size 12 on $R\Sigma_3^k$, $k = 5$ (Dimension = 8).
- Test statistic for comparing the extrinsic mean shapes = 36.56. (Abhishek(2008))
- p-value = $P(\chi_8^2 > 36.56) = 1.38 \times 10^{-5}$.

Glaucoma detection: extrinsic variation comparison

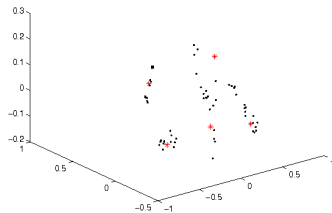
- Extrinsic sample variation for glaucoma induced eye = 0.038.
- Extrinsic sample variation for normal eye = 0.041.
- Test statistic for testing equality of extrinsic variations = -0.5572 . (Abhishek(2008))
- p-value = $P(|Z| > 0.5572) = 0.577$.

Glucoma detection plots: sample k -ads

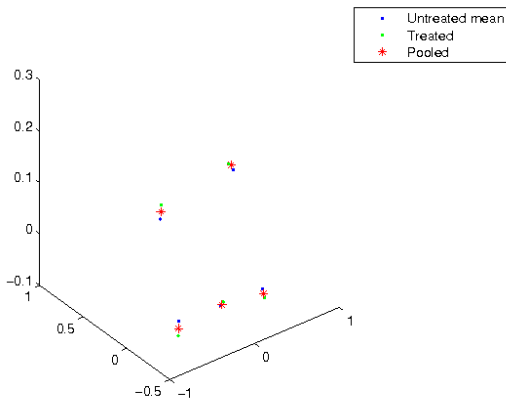
links for untrt eyes (black) along with the extrinsic mean (red)









links for trt eyes (black) along with the extrinsic mean (red)



Glaucoma detection plots: sample extrinsic means



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