Nonparametric Inference on Manifolds with Applications to Directional Data Analysis, Shape Analysis etc

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Based on the book *Nonparametric Statistics On Manifolds With Applications To Shape Spaces* jointly with R.N.Bhattacharya

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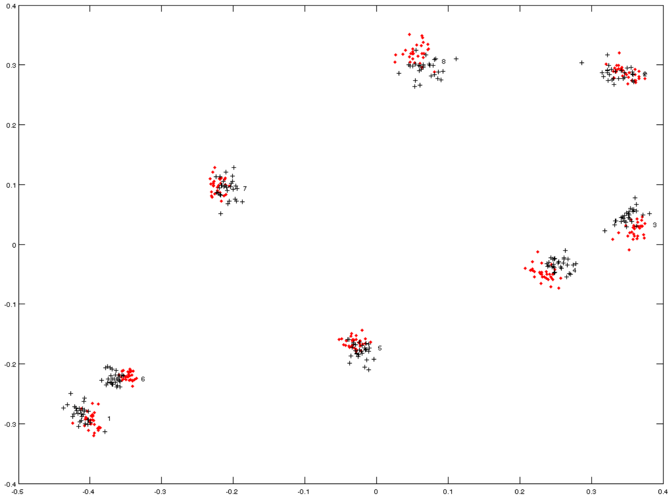
- Consider data on 2D image of gorilla skulls and their gender. There are 29 male and 30 female gorillas.
- Goal is to study the skull shapes and use that to detect difference in shapes between the sexes and predict the sex.
- This finds application in morphometrics and other biological sciences.
- Since different images obtained under different orientations, scale etc, it is important to be invariant to translations, rotations & scaling, i.e. use the skull shape.
- To get the skull shape, eight locations or landmarks are chosen on the midline plane of the skull images. The data can be found in *Dryden and Mardia, 98*.

Gorilla Skull Preshapes: Females (red), Males (+)

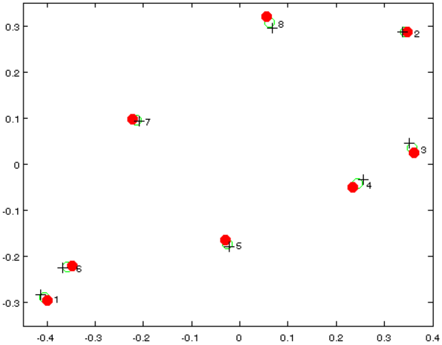


- Consider a configuration of k points or *landmarks* on a 2D image, not all same.
- This is called a *k-ad* in 2D. It can be represented by a $2 \times k$ real matrix or by a k-complex vector. For convinience, we will use the latter representation.
- The shape of this k-ad is its orbit or equivalance class under 2D translations, scaling and rotation.
- Hence two k-ads $z, w \in \mathbb{C}^k$ have the same shape if $w = se^{ir}z + t$ for some $t \in \mathbb{C}$, $s \in \mathbb{R}^+$, $r \in \mathbb{R}$.
- To study the shape of k-ad z, we may either remove the transformation effect, if possible, o.w. work with the orbit.
- To get rid of translation, substract the center of mass $\bar{z} = (1/k)\sum z_j$ from z.

- Standardize the centered k-ad to have complex norm 1, and removing the scale factor.
- The resulting centered normalized k-ad $z_p = (z - \bar{z})/\|z - \bar{z}\|$ is called a *preshape* of z. It contains shape information plus rotation.
- The set of all preshapes can be identified with the complex sphere $\mathbb{C}S^{k-2} \in \mathbb{C}^{k-1}$.

- The shape of preshape z_p is then the set $\{\lambda z_p : \lambda \in \mathbb{C}\}$, i.e. the complex line in $\mathbb{C}^{k-1}$ passing through the orgin and z_p.
- Hence the Planar Shape Space Σ_2^k or Kendall's (*Kendall, 1989*) Similarity Shape Space is the space of all complex lines passing through origin in $\mathbb{C}^{k-1}$.
- This space is the Complex Projective Space, a well known Riemannian manifold of real dimension $2k-4$.

Gorilla Skulls: Extrinsic Mean Shapes Plot



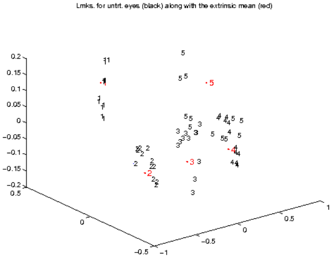
SAMPLE EX. MEANS FOR FEMALES (r.), MALES (+) ALONG WITH THE POOLED SAMPLE EX. MEAN (go)

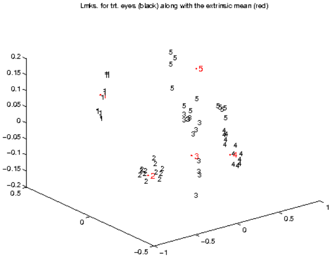
- When interested in the simalarity shape of k-ad z in three or higher dimensions, say m, we view $z \in M(m,k)$ as a $m \times k$ real matrix.
- The shape of z denoted by $\sigma(z)$ or $[z]$ is the set/orbit $\{[sRz_1 + t, \dots sRz_k + t] : s \in \mathbb{R}^+, R \in SO(m), t \in \mathbb{R}^m\}$, $SO(m)$ is the group of all $m \times m$ rotation matrices R ($RR' = I_m$, $\det(R) = 1$).
- To remove effects of translation and scaling, get the preshape z_p as before. Its shape is then $[z_p] = \{Rz_p : R \in SO(m)\}$.
- To make the resulting shape space Σ_m^k a manifold, consider only those k-ads whose preshapes have rank atleast $m-1$. Then Σ_m^k is a (not complete) Riemannian manifold of dimension $km - m - 1 - m(m-1)/2$.

- The reflection similarity shape of a $m \times k$ configuration z is its orbit under translation, scaling and all orthogonal transformations - rotations and reflection.
- Hence the shape $[z_p]$ of a preshape z_p is $\{Rz_p : R \in O(m)\}$ $(RR' = I_m)$.
- To make the resulting shape space a manifold, consider k-ads whose preshapes have rank m.
- Then $R\Sigma_m^k$ is a Riemannian manifold of dimension $km - m - 1 - m(m-1)/2$. It is locally like Σ_m^k

- Glaucoma is a major cause of eye blindness. Hence it is useful to find out if eye shape changes due to Galucoma and use that as a tool for disease detection.
- In this experiment 3D images of the Optic Nerve Head (ONH) of both eyes of 12 rhesus monkeys were collected. One of the eyes was treated to cause glaucoma, while the other was left untreated. Five landmarks were recorded on each eye.
- Hence a matched pair sample of size 12 on $R\Sigma_3^k \times R\Sigma_3^k$, $k = 5$, from some unknown distrubition.
- Goal is to test if the marginals of this distribution are identical.

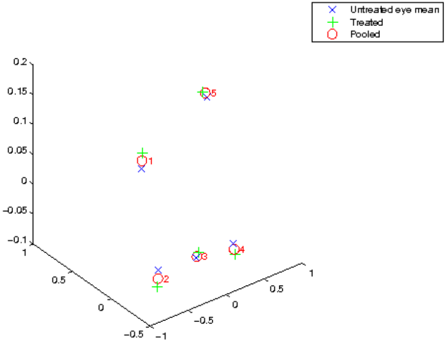
Glucoma detection plots: sample *k*-ads





5 LMKS. FROM NORMAL & INFECTED EYES OF 12 MONKEYS ALONG WITH THE SAMPLE EX. MEANS

Glaucoma Detection Plots: Sample Extrinsic Means

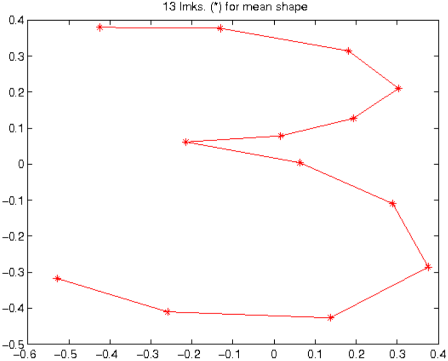


EX. MEAN SHAPES FOR THE 2 EYES ALONG WITH POOLED SAMPLE EX. MEAN

- When taking pictures with a camera, different amount of stretching may be applied in different directions. Then more appropriate to consider the affine shape.
- The *affine shape* of a k-ad z in $\mathbb{R}^m$ ($z \in M(m,k)$) is its orbit under all affine transformations, i.e., $[z] = \{(Az_1 + t, \dots, Az_k + t) : A \in GL(m), t \in \mathbb{R}^m\}$ with $GL(m)$ being the group of all n.s. linear transformations ($A \in M(m,m)$, $\det(A) \neq 0$).
- Then assuming that $z_c = z - \bar{z}$ has rank m and $k > m$, $[z]$ can be identified with the m-dimensional subspace of $\mathbb{R}^{k-1}$ spanned by the rows of z_c.
- This means that $A\Sigma_m^k$ is the space of all m-subspaces of $\mathbb{R}^{k-1}$, i.e. the Grassmanian (*Sparr, 1992*).
- It is a Riemannian manifold of dimension $mk - m - m^2$.

Application to Handwritten Digit recognition

- A random sample of 30 handwritten digit '3' were collected so as to devise a scheme to automatically classify handwritten characters. 13 landmarks were recorded on each image by *Anderson (1997)*.
- To analyse the affine shapes, we have iid sample of 30 on $A\Sigma_2^k$, $k = 13$.
- Goal is to estimate the distribution and use that to test if a given new subject is drawn from it.



EXTRINSIC MEAN SHAPE FOR THE HANDWRITTEN DIGIT 3 SAMPLE

- For projective shape analysis, we view the *k*-ad as a set of *k* rays passing through the orgin which is the camera hole.
- Hence the *k*-ad in this view is valued in the Real Projective Space $\mathbb{R}P^m$ - the space of all axis in $\mathbb{R}^{m+1}$.
- Elements of $\mathbb{R}P^m$ may be represented as equivalence classes $[x] = \{\lambda x : \lambda \in \mathbb{R}\}$, $x \in \mathbb{R}^{m+1} \setminus \{0\}$.
- Then a projective transformation α on $\mathbb{R}P^m$ is defined in terms of a $(m+1) \times (m+1)$ n.s. matrix A as $\alpha([x]) = [Ax]$. The group of all projective transformations on $\mathbb{R}P^m$ is denoted by $PGL(m)$.
- For a *k*-ad $y = (y_1, \ldots, y_k) \in (\mathbb{R}P^m)^k$, say $y_j = [x_j]$, $x_j \in \mathbb{R}^{m+1} \setminus \{0\}$, its *projective shape* is the set $\{(\alpha y_1, \ldots, \alpha y_k) : \alpha \in PGL(m)\}$, i.e. the orbit under $PGL(m)$.

Projective Shape Space $P\Sigma_m^k$

- To exclude singular shapes, define a k-ad y to be in *general position* if there exists a subset of $m+2$ landmarks such that the linear span of any $m+1$ points from this set is $\mathbb{R}P^m$, i.e., if the linear span of their representative points in $\mathbb{R}^{m+1}$ is $\mathbb{R}^{m+1}$.
- The space of shapes of all k-ads in general position is the projective shape $P\Sigma_m^k$.
- It is a Riemannian manifold of dimension $mk - \{(m+1)^2 - 1\} = mk - m(m+2)$.
- Registration based method of inference on this manifold has been considered in *Mardia and Patrangenaru (2005)*.

- When images/photos are obtained through a central projection, like a pinhole camera, projective shape analysis is useful.
- For images takes 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, similary shapes can be used.

- Let (M, ρ) be a metric space and Q be a prob. distn. on M.
- Given a continuous loss function f on $[0, \infty)$, consider the expected loss of Q:

$$F(p) = \int_M f(\rho(p, x))Q(dx), \;\; p \in M$$

- We call F the Frechet function of Q *Frechet, 1977*.
- The set of all minimizers of F is called the mean set of Q, denoted by C_Q.
- The minimum value is called the dispersion or spread of Q, denoted by V.
- Most studied case is the squared error loss, i.e. $f(\rho) = \rho^2$.

Given a iid sample from Q, define the sample mean set C_{Q_n} and sample dispersion V_n by replacing Q by the empirical Q_n, n being the sample size.

Theorem

If M is compact, given a iid sample, $C_{Q_n} \longrightarrow C_Q$ as $n \to \infty$ a.s.

Next we turn to non-compact spaces and restrict to loss functions of the type $f(u) = u^\alpha$, $u \geq 0$, $\alpha \geq 1$. Assume (1) every closed and bounded subset of M is compact and (2) The Frechet function $F(p)$ is finite for some $p \in M$.

Theorem

If (1) and (2) hold with $f(u) = u^\alpha$, the mean set C_Q of Q is non-empty and compact. Further, given a iid sample, $C_{Q_n} \longrightarrow C_Q$ as $n \to \infty$ a.s.

- Define the sample mean μ_n as any measurable selection from the sample mean set.
- In view of the theorems before, it is a consistent estimate of the mean μ of Q (if μ exists i.e. C_Q is a singleton).

Theorem

Also under the theorems' assumptions, the sample dispersion V_n is a consistent estimator of the dispersion V of Q (even if μ is not defined).

Let M be a d-dimensional differentiable manifold and ρ a distance metrizing the topology of M.
Assume
A1 Q has a unique mean μ.
A2 Q has support in a single coordinate patch (U, ϕ) $(\phi : U \to \mathbb{R}^d)$.
A3 For all $x \in \mathbb{R}^d$, $y \mapsto h(x, y) = f \circ \rho(\phi^{-1}(x), \phi^{-1}(y))$ is twice continuously differentiable in a neighborhood of $y = \phi(\mu)$.
A4 For $X \sim Q$, $E\|Dh\big(\phi(X), \phi(\mu)\big)\|^2 < \infty$.
A5 $E\{\sup_{|y_1 - y_2| < \epsilon} |D_s D_r h(\phi(X), y_1) - D_s D_r h(\phi(X), y_2)|\} \longrightarrow 0$ as $\epsilon \to 0$ forall r, s.
A6 $\Lambda = ((E\{D_s D_r h(\phi(X), \phi(\mu))\}))$ is nonsingular.

Theorem

*(a) Let μ_n denote a sample mean. Under assumptions **A1-A6**,*

$$\sqrt{n}(\phi(\mu_n) - \phi(\mu)) \xrightarrow{d} N_d\left(0, \Lambda^{-1}\Sigma(\Lambda')^{-1}\right).$$

(b) Let V_n and V be the sample and population dispersion respectively. Under further assumption $var\{f \circ \rho(X, \mu)\} < \infty$,

$$\sqrt{n}(V_n - V) \xrightarrow{d} N\left(0, var(f \circ \rho(X, \mu))\right).$$

Therefore we can construct asymptotic and bootstrap Confidence region/interval for the population mean and dispersion.

- When M is embedded in a high dimensional Euclidean space and the distance induced from this embedding is used to define the mean and dispersion, the corresponding statistical analysis is called Extrinsic Analysis.
- Any injective map whose derivative is also injective is an embedding.
- When M is a Riemannian manifold and the geodesic distance is used instead, we perform Intrinsic Analysis on the manifold.
- Unless specified o.w., we deal with squared distance loss, i.e. $F(p) = \int_M \rho^2(p, x) Q(dx)$.

- Let (M, g) be a complete connected Riemannian manifold of dimension d with metric tensor g which induces a distance namely the geodesic distance on M.
- Geodesics are curves on M having 0 accelaration. They are locally length minimizing.
- The exponential map is defined as, for $p \in M$, $v \in T_p(M)$ as $\exp_p(v) = \gamma(1)$, γ being a geodesic staring at p with starting velocity v.
- Define the cut locus $C(p)$ of p as the set of points $\gamma(t0)$, where γ is a unit speed geodesic starting at p and $t0$ is the sup of all $t > 0$ s.t γ is distance minimizing from p to $\gamma(t)$.

- Sectional Curvature Consider a 2D subspace π of T_pM. A 2D submanifold of M is swept out by the set of all geodesics starting at p and with initial velocities lying in π. The Gaussian curvature of this submanifold is called the sectional curvature at p of the section π.
- The injectivity radius $inj(M)$ of M is $\inf\{d_g(p, C(p)) \colon p \in M\}$.
- Let $r_* = \min\{\mathrm{inj}(M), \pi/\sqrt{C}\}$, where C is the least upper bound of sectional curvatures of M.
- Normal Coordinates The exponential map at p is injective on $\{v \in T_p(M) \colon \|v\| < r_*\}$. Its inverse defines a coordinate system called normal coordinates.

- If the support of Q is in a geodesic ball of radius $r_*/4$, i.e. $\mathrm{supp}(Q) \subseteq B(p, r_*/4)$, then Q has a unique intrinsic mean (*Karchar, 1977 and Le, 2001*).
- *Kendall, 1990* has shown that if $\mathrm{supp}(Q) \subseteq B(p, r_*/2)$, then there is a unique intrinsic mean in that ball, say μ_I.
- In that case, the local sample intrinsic mean in $B(p, r_*/2)$ is a strongly consistent estimator of μ_I.

Theorem

Suppose $\mathrm{supp}(Q) \subseteq B(\mu_I, r_*/2)$, μ_I *being the local intrinsic mean of Q. Let* μ_{nI} *be the sample int. mean in* $B(\mu_I, r_*/2)$ *from* $X_1, \ldots, X_n$ *iid Q. Let* $x_j = \phi(X_j) = \exp_{\mu_I}^{-1}(X_j)$ *be the normal coordinates of the sample. Then* $E(x_1) = 0$ *and*

$$\sqrt{n}\phi(\mu_{nI}) \xrightarrow{d} N\big(0, \Lambda^{-1}\Sigma\Lambda^{-1}\big)$$

where $\Sigma = 4E(x_1 x_1')$ *and in case M has constant curvature C,* Λ *equals*

$$\Lambda_{rs} = 2E\Big\{\frac{1 - g(|x_1|)}{|x_1|^2} x_1^r x_1^s + g(|x_1|)\delta_{rs}\Big\},\ 1 \leq r, s \leq d,$$

$$g(y) = \begin{cases} 1 & \text{if } C = 0 \\ \sqrt{C}y\cos(\sqrt{C}y)/\sin(\sqrt{C}y) & \text{if } C > 0 \\ \sqrt{-C}y\cosh(\sqrt{-C}y)/\sinh(\sqrt{-C}y) & \text{if } C < 0. \end{cases}$$

- The sample int. mean μ_{nI} satisfies $(1/n)\sum_{i=1}^{n} \exp_{\mu_{nI}}^{-1}(X_i) = 0$.
- Hence is a fixed point of $f\colon M \to M$, $f(p) = \exp_p\left\{(1/n)\sum_{i=1}^{n} \exp_p^{-1}(X_i)\right\}$.
- Using this, we can build a fixed point algorithm to compute μ_{nI}. This is derived in *Le(2001)*.

- Given two indep. samples coming from, say, Q_1 and Q_2, we can construct two sample tests to compare the sample means and dispersions and hence distinguish between Q_1 and Q_2.
- Let μ_j, Σ_j, V_j and σ_j denote the int. parameters specific to Q_j and $\hat{\mu}_j$, $\hat{V}_j$,.. be their sample analogues, such that

$$\sqrt{n_j}\exp_{\mu_j}^{-1}(\hat{\mu}_j) \xrightarrow{d} N_d(0,\Sigma_j), \ \sqrt{n_j}(\hat{V}_j - V_j) \xrightarrow{d} N(0,\sigma_j^2).$$

Then

$$n(\phi(\hat{\mu}_1)-\phi(\hat{\mu}_2))'\left(\hat{\Sigma}_1/n_1+\hat{\Sigma}_1/n_2\right)^{-1}(\phi(\hat{\mu}_1)-\phi(\hat{\mu}_2)) \xrightarrow{d} \mathcal{X}_d^2,$$

$\phi = \exp_{\hat{\mu}}^{-1}$, $\hat{\mu}$ the pooled sample int. mean., if $H_0 : \mu_1 = \mu_2$ holds.
- Similarly under the null $V_1 = V_2$,

$$(\hat{V}_1 - \hat{V}_2)/\sqrt{\sum_{j=1}^{2}\hat{\sigma}_j^2/n_j} \xrightarrow{d} N(0,1).$$

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

- It is a Riemannian manifold of dim. d.
- $T_pS^d = \{v \in \mathbb{R}^{d+1} : p'v = 0\}$
- Geodesics are great circles

$$\gamma_{p,v}(t) = \cos(t\|v\|)p + \sin(t\|v\|)v/\|v\|, \; t \in \mathbb{R}.$$

- The inverse-exponential map $\exp_p^{-1} : S^d \setminus \{-p\} \to \{v \in T_p : \|v\| < \pi\}$ given by

$$\exp_p^{-1}(q) = \frac{\mathrm{acos}(p'q)}{\sqrt{1-(p'q)^2}}\{q - (p'q)p\}.$$

- The geodesic distance between p, q equals $\mathrm{acos}(p'q)$.

- Consider data on 2D image of gorilla skulls and their gender. There are 29 male and 30 female gorillas.
- Goal is to study the skull shapes and use that to detect difference in shapes between the sexes and predict the sex.
- This finds application in morphometrics and other biological sciences.
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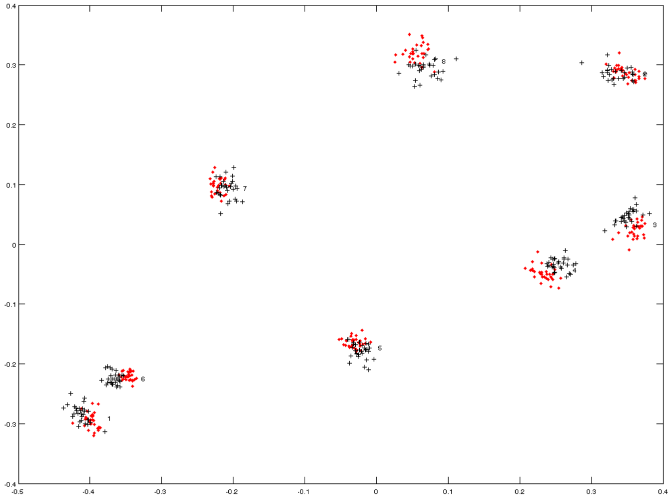
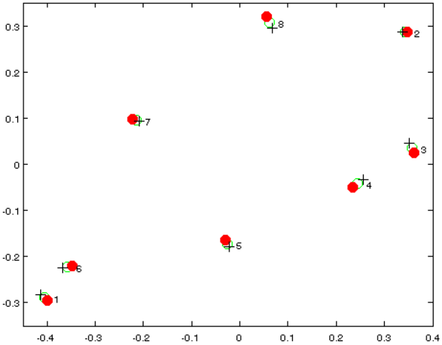
- To get the skull shape, eight locations or landmarks are chosen on the midline plane of the skull images. The data can be found in *Dryden and Mardia, 98*.

Gorilla Skull Preshapes: Females (red), Males (+)



Gorilla Skulls: Extrinsic Mean Shapes Plot

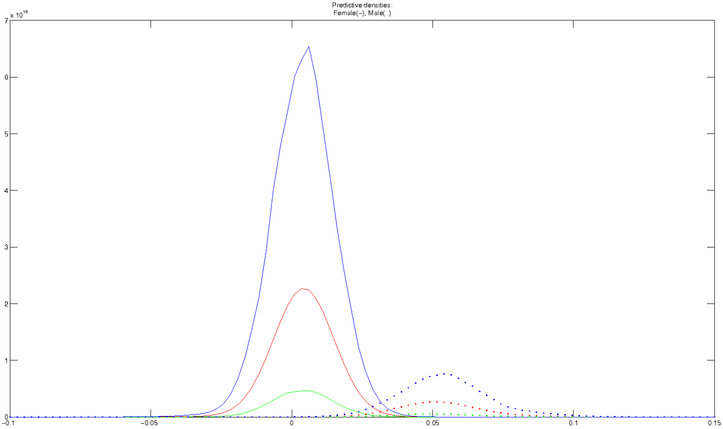


SAMPLE EX. MEANS FOR FEMALES (r.), MALES (+) ALONG WITH THE POOLED SAMPLE EX. MEAN (go)

- The geodesic distance between the intrinsic and extrinsic means is 5.54×10^{-7} for the female sample and 1.96×10^{-6} for males.
- The two sample test statistic for comparing the intrinsic mean shapes equals 391.63 and the asymptotic p-value for the chi-squared test is $P(\mathcal{X}_{12}^2 > 391.63) < 10^{-16}$.
- P-value estimated using pivotal b.s. method using 10^5 simulations is 0.
- A parametric test in *Dryden & Mardia (1998), pp. 168-172* has a p-value of 10^{-4}.
- The sample extrinsic dispersions for female and male samples are 0.0038 and 0.005 respectively.
- The two sample test statistic for testing equality of extrinsic dispersions equals 0.923, and the asymptotic p-value is $P(N(0,1) > 0.923) = 0.356$.

- The shape density for the two distributions are estimated independently by nonparametric Bayesian methods.
- Here is a 1D slice of the density estimates for the male and female gorrilas.
- Densities evaluated along the geodesic starting at the female towards the male sample ex. mean.

Female: solid, Male: dotted, Posterior mean densities: red, 95% C.R.: blue/green



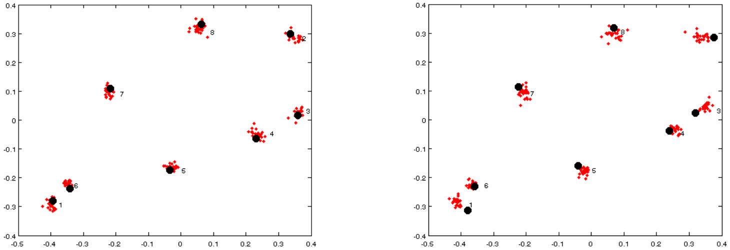
- From the shape density estimates, we can predict the gender from the shape via np discriminant analysis.
- Assumed the unconditional probability of being female is 0.5.
- Letting $f_1(m)$ and $f_2(m)$ denote the female and male shape densities, the conditional probability of being female given shape data $\sigma(z)$ is $p(\sigma(z)) = 1/\{1 + f_2(\sigma(z))/f_1(\sigma(z))\}$.
- To test the performance of the classifier, randomly partition the sample into training-test samples, using training samples, get the classifier and apply it to the test data.

This table presents the estimated posterior probabilities of being female for each gorilla in the test sample along with a 95% credible interval (CI) for $p([z])$ for one such partition. Also shown is the ex. dist. between the sample shape and the female($\hat{\mu}_1$), male($\hat{\mu}_1$) sample ex. means.

gender	$\hat{p}([z])$	95% CI	$d_E([z], \hat{\mu}_1)$	$d_E([z], \hat{\mu}_2)$
F	1.000	(1.000,1.000)	0.041	0.111
F	1.000	(0.999,1.000)	0.036	0.093
F	0.023	(0.021, 0.678)	0.056	0.052
F	0.998	(0.987, 1.000)	0.050	0.095
F	1.000	(1.000, 1.000)	0.076	0.135
M	0.000	(0.000, 0.000)	0.167	0.103
M	0.001	(0.000, 0.004)	0.087	0.042
M	0.992	(0.934, 1.000)	0.091	0.121
M	0.000	(0.000, 0.000)	0.152	0.094

- There is misclassification in the 3rd female and 3rd male.
- Based on the CI, there is some uncertainity in classifying the 3rd female.
- Perhaps there is something unusual about the shapes for these individuals, which was not represented in the training data, or they were labelled incorrectly.
- Can also define a distance-based classifier, which allocates a test subject to the group having mean shape closest to that subjects' shape.
- The 2 classifiers give consistent results.
- However, such a classifier may be sub-optimal in not taking into account the variability within each group.
- In addition, the approach is deterministic and there is no measure of uncertainty in classification.

Gorilla Skull Training and Test Samples



Training(red) & mis-classified test(black) samples corresponding to females (left) & males (right).

- Let M be a d-dim. differentiable manifold embedded in a D-dim. Euclidean space E, $\pi : M \to E$ be the embedding.
- Let ρ be the distance metric inherited via the embedding: $\rho(p, q) = \|\pi(p) - \pi(q)\|$.
- Use that to define the extrinsic mean and dispersion of a probability Q on M as minimizers and minimum value of the Frechet function

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

- For $\tilde{\mu} \in E$, its projection into M is the set

$$P_M(\tilde{\mu}) = \{x \in M\colon \|\tilde{\mu} - \pi(x)| \leq \|\tilde{\mu} - \pi(y)|\forall y \in M\}$$

which is non-empty if $\pi(M)$ is closed.
- If this set is a singleton, μ is said to be non-focal.

Theorem

(a) The extrinsic mean set of Q is the projection set $P_M(\tilde{\mu})$, $\tilde{\mu} = \int xQ \circ \pi^{-1}(dx)$. (b) The extrinsic dispersion equals $\|\tilde{\mu} - M\|^2 + \int \|x - \tilde{\mu}\|^2 Q \circ \pi^{-1}(dx)$. (c) The extrinsic mean μ_E exists iff $\tilde{\mu}$ is non-focal.

- Embedding π = Inclusion map, Extrinsic distance d_E = Chord distance.
- $\tilde{\mu} = \int_{S^d} xQ(dx) \in \mathbb{R}^{d+1}$.
- Extrinsic mean

$$\mu_E = \pi^{-1}(P_{S^d}(\tilde{\mu})) = \frac{\tilde{\mu}}{\|\tilde{\mu}\|}$$

  exists iff $\tilde{\mu} \neq 0$.
- Extrinsic dispersion $V = 2(1 - \|\tilde{\mu}\|)$.

- Let $\mu_E = \pi^{-1}P(\tilde{\mu})$ be the ex. mean and V the dispersion of Q. ($\tilde{\mu} = \mathrm{E}(Q \circ \pi^{-1})$).
- Let $X_1, \ldots, X_n$ be the image of the sample $x_1, \ldots, x_n$ under embedding π.
- Then sample ex. mean $\mu_{nE} = \pi^{-1}P(\bar{X})$ where $\bar{X} = (1/n)\sum_{i=1}^{n} X_i$. Let V_n denote the sample ex. dispersion. Then

$$\sqrt{n}(\pi(\mu_{nE}) - \pi(\mu_E)) = \sqrt{n}(P(\bar{X}) - P(\tilde{\mu})) = \sqrt{n} d_{\tilde{\mu}} P(\bar{X} - \tilde{\mu}) + o_P(1),$$
$$\sqrt{n}(V_n - V) = \frac{1}{\sqrt{n}} \sum \{\rho^2(x_i, \mu_E) - V\} + o_P(1)$$

which proves

Theorem

If $\tilde{\mu}$ is non-focal, P is continuously diffble in a neighborhood of $\tilde{\mu}$ and $E\{\rho^4(x_1)\} < \infty$, then

$$\sqrt{n}(\pi(\mu_{nE}) - \pi(\mu_E), V_n - V) \xrightarrow{L} N_{d+1}(0, \Sigma)$$

Among the possible embeddings, we seek out equivariant embeddings which preserve many of the geometric features of M.

Definition

For a Lie group H acting on M, an embedding $\pi : M \to \mathbb{R}^D$ is H-equivariant if there exists a injective group homomorphism $\phi : H \to GL(D, R)$ such that

$$\pi(hp) = \phi(h)\pi(p) \ \forall p \in M, \ \forall h \in H.$$

Here $GL(D, R)$ is the general linear group of all $D \times D$ non-singular matrices.

- $P : R^{d+1} \to S^d$, $P(\tilde{\mu}) = \tilde{\mu}/\|\tilde{\mu}\|$.
- $d_{\tilde{\mu}}P : R^{d+1} \to T_{P(\tilde{\mu})}S^d$, $d_{\tilde{\mu}}P(x) = J(\tilde{\mu})x$, $J = \|\tilde{\mu}\|^{-1}\left(I_{d+1} - \|\tilde{\mu}\|^{-2}\tilde{\mu}\tilde{\mu}'\right)$.
- $\sqrt{n}(\bar{x}/\|\bar{x}\| - \mu_E) \xrightarrow{L} N_{d+1}(0, J\mathrm{Cov}(x_1)J')$.
- Hence

$$\{n\|\bar{x}\|^2(\mu_{nE} - \mu_E)'B(B'SB)^{-1}B'(\mu_{nE} - \mu_E) \leq \mathcal{X}^d(0.95)\}$$

  gives a 95% asymptotic C.R. for μ_E.
- Here B is an orthonormal basis for $T_{\mu_{nE}}S^d$ ($B'\bar{x} = 0$, $B'B = I_d$) and $S = 1/n\sum(x_i - \bar{x})(x_i - \bar{x})'$.
- For $p_0 \in S^d$, $p \in R^{d+1}$, $B(p_0)'p$ are the (isometric) coord. of linear projection of p into $T_{p_0}S^d$.

- Given two sample $\mathbf{x}_1, \mathbf{x}_2$, the $\mathcal{X}_d^2$ test statistic for testing $H_0 : \mu_{1E} = \mu_{2E}$ given by

$$\|\hat{\mu}_{1E} - \hat{\mu}_{2E}\|^2_{B\hat{\Sigma}^{-1}B'},$$

B being an o.n. basis for the tangent space at the pooled sample mean $\bar{x}$, $\|x\|^2_A = x'Ax$,

$$\hat{\Sigma} = B'\{\sum_{j=1}^{2} n_j^{-1}|\bar{x}_j|^{-2}\|I_{d+1} - |\bar{x}_j|^{-2}\bar{x}_j\bar{x}_j'\|_{S_j}\}B.$$

- The bootstrap p-value given by

$$Pr(\|\mu^*_{1E} - \mu^*_{2E} - \hat{\mu}_{1E} + \hat{\mu}_{2E}\|_{B\Sigma^{*-1}B'} > \|\hat{\mu}_{1E} - \hat{\mu}_{2E}\|_{B\hat{\Sigma}^{-1}B'} \big| x).$$

- From the recent lava flow of 1947-48, 9 specimens on the directions of flow were collected.
- The data can be viewed as an iid sample on S^2 and can be found in *Fisher(1953)*.
- The sample extrinsic and intrinsic means are very close, at a geodesic distance of 0.0007 from each other.
- They are $\hat{\mu}_E = (0.2984, 0.1346, 0.9449)'$ and $\hat{\mu}_I = (0.2990, 0.1349, 0.9447)'$ respectively.

- The asymptotic C.R. for the population extrinsic mean turns out to be

$$\{p \in S^2 \colon p'\bar{x} > 0,\ n|\bar{x}|^2 p'B(B'SB)^{-1}B'p \leq \mathcal{X}_2^2(0.95) = 5.9915\}.$$

- In *Fisher(1953)*, a von-Mises-Fisher distribution is fitted to the data and a 95% C.R. based on the MLEs is obtained for the mean direction of flow (extrinsic or intrinsic). It is

$$\{p \in S^2 \colon d_g(\hat{\mu}_E, p) \leq 0.1536\}.$$

- The latter nearly contains the former and is considerably larger.

- We also derive 95% C.R.s for the intrinsic mean. The symetric C.R. is

$$\{\mu_I : d_g(\mu_I, \hat{\mu}_I) \leq 0.1405\}.$$

- The ellipsoidal region becomes

$$\{\mu_I : n\phi(\mu_I)'\hat{\Lambda}\hat{\Sigma}^{-1}\hat{\Lambda}\phi(\mu_{nI}) \leq 5.992\}$$

where ϕ gives normal coordinates into $T_{\hat{\mu}_I}S^2$ (identified with R^2).

- $M = \Sigma_2^k = N/G$,
  $N = \{p \in C^k : \sum p_j = 0, \|p\| = 1\} \equiv S^{2k-3}$,
  $G = \{e^{i\theta} : \theta \in R\} \equiv S^1$.
- $T_{[p]}M = \{v \in C^k \colon\ v'1 = 0,\ v'p = 0\}$.
- The map $\sigma : N \to M$ is a Riemannian submersion. Its derivative is sujective and a isometry.
- The exponential map Exp given by $Exp_{[p]} : T_{[p]} \to \Sigma_2^k$, $Exp_{[p]} = \sigma \circ \exp_p \circ d\sigma_{[p]}^{-1}$, exp denoting the exponential map on the sphere S^{2k-3}.
- The geodesic distance between two shapes $[x]$ and $[y]$ is given by

$$d_g([x],[y]) = \inf_{\theta \in (-\pi,\pi]} d_{gs}(x, e^{i\theta} y)$$

$$= \inf \arccos(Re(e^{-i\theta}\bar{y}'x)) = \arccos(|\bar{y}'x|).$$

- Its sectional curvatures lie between 1 & 4.
- It has an injectivity radius of $\pi/2$, $r_* = \pi/2$.
- The inverse-exponential map/ normal coordinates $Exp_{[p]}^{-1} : B_M(p, \pi/2) \to T_{[p]} \equiv C^{k-2}$ w.r.t. an orthonormal basis $\{v_1, \ldots, v_{k-2}\}$ are

$$\phi(q) = (z_1, \ldots, z_{k-2})', \; z_j = \frac{r}{\sin(r)} e^{i\theta} \bar{v}_j' q$$

where $r = d_g([p], [q])$, $e^{i\theta} = \bar{q}'p/|\bar{q}'p|$.

- $B_M([p], \pi/2)$ is $\Sigma_2^k \setminus C([p])$,

$$C([p]) = \{[q] : d_g(\pi(p), \pi(q)) = \pi/2\} = \{\pi(q) : \bar{q}'p = 0\}.$$

- Q has unique (local) intrinsic mean μ_I if its support in a open geodesic ball of radius $r_*/2 = \pi/4$.
- Then
$$\sqrt{n}\phi(\hat{\mu}_I) \xrightarrow{L} N_d(0, \Lambda^{-1}\Sigma\Lambda^{-1})$$
if Λ is non-singular.
- Let $X \sim Q$ and $\tilde{X} \equiv \phi(X) = (\tilde{X}_1, \ldots, \tilde{X}_{2k-4})$ be its normal coordinates at μ_I.
- Then $\Sigma = 4\mathrm{E}(\tilde{X}\tilde{X}')$ is positive if for example Q has a density.

Theorem

- $\Lambda = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{12}' & \Lambda_{22} \end{bmatrix}$ *where*
- $(\Lambda_{11})_{rs} = 2\mathrm{E}\Big[\, d\cot(d)\delta_{rs} - \frac{(1-d\cot(d))}{d^2}(\mathrm{Re}(\tilde{X}_r))(\mathrm{Re}(\tilde{X}_s)) + \frac{\tan(d)}{d}(\mathrm{Im}(\tilde{X}_r))(\mathrm{Im}(\tilde{X}_s))\,\Big]$,
- $(\Lambda_{22})_{rs} = 2\mathrm{E}\Big[\, d\cot(d)\delta_{rs} - \frac{(1-d\cot(d))}{d^2}(Im\tilde{X}_r)(Im\tilde{X}_s) + \frac{tan(d)}{d}(Re\tilde{X}_r)(Re\tilde{X}_s)\,\Big]$,
- $(\Lambda_{12})_{rs} = -2\mathrm{E}\Big[\, \frac{(1-d\cot(d))}{d^2}(\mathrm{Re}(\tilde{X}_r))(\mathrm{Im}(\tilde{X}_s)) + \frac{\tan(d)}{d}(\mathrm{Im}(\tilde{X}_r))(\mathrm{Re}(\tilde{X}_s))\,\Big]$ *with* $d = d_g(X, \mu_I)$.
- *If* $\mathrm{supp}(Q) \subseteq B(\mu_I, R)$, *then* Λ *is positive definite, where* R *is the unique solution of* $\tan(R) = 2R$ *in* $(0, \frac{\pi}{2})$.
- R *is approximately* 0.37101π.

- A 95% C.R. for μ_I given by

$$\{n\hat{\phi}(\mu_I)'\hat{\Lambda}\hat{\Sigma}^{-1}\hat{\Lambda}\hat{\phi}(\mu_I) < \mathcal{X}^2_{2k-4}(0.95)\},$$

  $\hat{\phi}$ denoting normal-coordinates in $T_{\hat{\mu}_I}$ or

- $$\{nd_g^2(\mu_I, \hat{\mu}_I) \leq \sum_{j=1}^{2k-4} \lambda_j Z_j^2\},$$

  λ_js being eigen-values of $\hat{\Lambda}^{-1}\hat{\Sigma}\hat{\Lambda}^{-1}$ while Z_j iid N(0,1).

- $nd_g^2(\mu_I, \hat{\mu}_I) = n\|\phi(\hat{\mu}_I)\|^2$.

- Can be embedded into space of $k \times k$ complex Hermitian matrices $S(k, C)$ via the Veronese-Whitney embedding $\pi([z]) = zz^*$.
- It induces the extrinsic distance $d_E([u], [v]) = \|\pi([u]) - \pi([v])\| = \sqrt{2(1 - |u^* v|^2)}$.
- Let $\tilde{\mu}$ denote the Euclidean mean of $Q \circ \pi^{-1}$. It is in $S(k, C)$, has eigen values in $[0, 1]$ adding to 1, has complex rank atleast one.

Theorem

The projection set of $\tilde{\mu}$ into Σ_2^k is the set of eigen-rays corresponding to its largest eigen-value λ. Hence the extrinsic mean is well defined iff λ has multiplicity 1. The extrinsic dispersion equals $2(1 - l)$.