STATISTICS ON SHAPE MANIFOLDS: THEORY AND APPLICATIONS

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CONTENTS

- 1. INTRODUCTION - EXAMPLES
- 2. PROBAB. MEASURES ON MANIFOLDS
  (a) FRÉCHET MEAN
  (b) EXTRINSIC MEAN
  (c) INTRINSIC MEAN
  (d) ASYMP. DISTR. OF SAMPLE MEANS
- 3. SHAPES OF k-ADS
  (a) KENDALL'S SPACES: Σ_m^k
  (b) REFLECTION SHAPE SPACES: $R\Sigma_m^k$
  (c) AFFINE SHAPE SPACES: $A\Sigma(m, k)$
  (d) PROJECTIVE SHAPE SPACES: $P\Sigma(m, k)$
- 4. NONPARAMETRIC TESTS

1. INTRODUCTION - EXAMPLES

- (1) DIRECTIONAL STATISTICS: $M = S^2$. PALEOMAGNETISM, DIRECTION OF A SIGNAL.
- (2) AXIAL STATISTICS: $M = \mathbb{R}P^2$. LINES OF GEOLOGICAL FISSURES, AXES OF CRYSTALS, OBSERVATIONS ON GALAXIES.
- (3) KENDALL SHAPE SPACES (OF k-ADS): $M = \Sigma(m, k) \approx S^{mk-m-1}/SO(m)$. MORPHOMETRICS (BOOKSTEIN), MEDICAL IMAGING, ARCHAEOLOGY.

- (4) REFLECTION SHAPE SPACES (OF k-ADS): $M = \mathbb{R}\Sigma(m, k) \approx S^{mk-m-1}/O(m)$.
- (5) AFFINE SHAPE SPACES (OF k-ADS): $M = A\Sigma(m, k)$. SCENE RECOGNITION AND RECONSTRUCTION, CARTOGRAPHY, PATTERN RECOGNITION, BIOINFORMATICS.
- (6) PROJECTIVE SHAPE SPACES (OF k-ADS): $M = P\Sigma(m, k)$. MACHINE VISION, ROBOTICS.

2(a)

- ASSUMPTION: CLOSED BOUNDED SUBSETS OF (M, ρ) ARE COMPACT.
- **FRÉCHET** FUNCTION OF A PROBAB. Q IS

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

- FRÉCHET MEAN SET IS THE SET OF MINIMIZERS OF F. A UNIQUE MINIMIZER IS CALLED THE FRÉCHET MEAN OF Q, SAY μ_F. SAMPLE FRÉCHET MEAN μ_n, F IS A MEASURABLE SELECTION FROM THE MEAN SET OF THE EMPIRICAL Q_n BASED ON I.I.D. $X_1, \ldots, X_n \sim Q$.
- **PROPOSITION 1**. LET F BE FINITE. (i) THEN THE FRÉCHET MEAN SET IS NONEMPTY COMPACT. (ii) IN CASE OF A UNIQUE MINIM. μ_F, $\mu_{n,F} \to \mu_F$ (WITH PROBAB. ONE). (ZIEZOLD,1977; BP,2003).

2(b). EXTRINSIC MEAN μ_E OF Q

- M: COMPLETE (d-DIM.) DIFF. MANIFOLD. THE METRIC $\rho = \rho_E$ IS INDUCED BY AN EMBEDDING $J : M \to \mathbb{R}^N$.
- μ^J = MEAN OF IMAGE Q^J OF Q in $\mathbb{R}^N$.
- μ_E = PROJECTION OF μ^J ON $J(M)$ (IF UNIQUE) IS EXTRINSIC MEAN OF Q.
- EXAMPLE.

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

J = INCLUSION MAP, ρ_E = CHORD DISTANCE, μ_E = UNIQUE IFF $\mu^J \neq 0$ ($\in \mathbb{R}^{d+1}$).

- **PROPOSITION 2.** SUPPOSE Q^J HAS FINITE SECOND MOMENTS, AND μ_E IS UNIQUE. THEN THE PROJECTION OF $\mu_{n,E}$ ON THE TANGENT SPACE $T_{\mu_E}M$ AT μ_E IS ASYMP. GAUSSIAN $N(0, \Gamma/n)$. $\square$ (EQUIVARIANT EMBEDDING DESIRABLE)
- **EQUIVARIANT EMBEDDING.** G (LIE) GROUP ACTING ON M, $J : M \to \mathbb{R}^N$ EMBEDDING IS G-EQUIVARIANT IF THERE EXISTS A GROUP HOMOMORPHISM $\phi : G \to GL(N, \mathbb{R})$ SUCH THAT

$$J(gp) = \phi(g)J(p) \;\; \forall p \in M, \;\; g \in G.$$

2(c). INTRINSIC MEAN μ_I OF Q

- M: COMPLETE RIEMANNIAN MANIFOLD, METRIC TENSOR g, $\rho = \rho_g$ GEODESIC DIST.
- INTRINSIC MEAN OF Q IS μ_I = MINIMIZER OF F, IF UNIQUE.
- TERMS: (i) $\gamma(t)$ IS A GEODESIC IF $(\mathrm{D}^2/\mathrm{dt}^2)\gamma(t) = 0$ (ZERO ACCELERATION).
  (ii) CUT LOCUS OF p (CUT(p)).
  (iii) INJECTIVITY RADIUS (INJ(M)).
  (iv) Exp_p ($T_pM \to M$): $\mathrm{Exp}_p(v) = \gamma(1)$, γ GEODESIC, $\gamma(0) = p$, $\dot\gamma(0) = v$.
  (v)
$$\mathrm{Log}_p = \mathrm{Exp}_p^{-1} : M \setminus \mathrm{CUT}(p) \to T_pM.$$
  (vi) SECTIONAL CURVATURE AT p .
- EXAMPLE. $M = S^d$. GEODESICS ARE GREAT CIRCLES, ρ_g IS ARC DISTANCE. CUT(p) = $\{-p\}$. INJ(M) = π.

- $$\mathrm{Exp}_p(v) = cos(|v|)p + sin(|v|)\frac{v}{\|v\|},\ (v \neq 0).$$

- $$Log_p(x) = (1-(p\cdot x)^2)^{-1/2}\arccos(p\cdot x)(x-(p\cdot x)p),\ x \neq p.$$

- SECTIONAL CURVATURE = 1 (CONSTANT)
- LET C DENOTE THE L.U.B. OF SECTIONAL CURVATURES ON M IF L.U.B > 0, AND $C = 0$ IF $L.U.B. \leq 0$.
$$r^* := min\{INJ(M), \pi/\sqrt{C}\}.$$
- **PROPOSITION 3**. IF SUPP(Q) $\subset B(p, r^*/2)$, THERE EXISTS A UNIQUE INTRINSIC MEAN μ_I OF Q ON THE METRIC SPACE $\overline{B(p, r^*/2)}$. IF SUPP(Q) $\subset B(p, r^*/4)$, THEN μ_I IS THE INTRINSIC MEAN OF Q ON M. □ (KARCHER,1977;KENDALL,1990)

- **PROPOSITION 4.** (a) ASSUME SUPP(Q) $\subset B(p, r^*/2)$, $Q(CUT(p)) = 0$. THEN $Log_{\mu_I}(\mu_{n,I})$ IS ASYMP. GAUSSIAN $N(0, \Gamma/n)$.
(b) SUPPOSE (i) Q IS ABS. CONT., (ii) THE INTRINSIC MEAN μ_I EXISTS, (iii) F is TWICE CONT. DIFF. IN A NBD. OF μ_I. THEN $Log_{\mu_I}(\mu_{n,I})$ IS ASYMP. GAUSSIAN $N(0, \Gamma/n)$.
□

- IN NORMAL COORDINATES (UNDER Log_{μ_I}), WITH THE IMAGE Q_L OF Q, ONE HAS

$$\int_{T_{\mu_I}M} vQ_L(dv) = 0,\ \Gamma = \Lambda^{-1}\Sigma\Lambda^{-1},$$

$$[\Sigma = COV(Q_L),\ \Lambda = (\text{HESSIAN OF F AT } \mu_I) \geq K] \qquad (*)$$

$$K_{ij} = \int [2(\left(\frac{1 - f(|v|)}{|v|^2}\right) v^i v^j + f(|v|)\delta_{ij})]Q_L(dv);$$

- $$f(r) = \begin{cases} 1 & \text{if } C = 0 \\ \sqrt{C}r\frac{cos(\sqrt{C}r)}{sin(\sqrt{C}r)} & \text{if } C > 0 \\ \sqrt{-C}r\frac{cosh(\sqrt{-C}r)}{sinh(\sqrt{-C}r)} & \text{if } C < 0 \end{cases}$$
- THERE IS EQUALITY IN (*) IF M HAS CONSTANT SECTIONAL CURVATURE.

3. SHAPE SPACES M OF k-ADS

- EACH OBSERVATION $\mathbf{x} = (x_1, \ldots, x_k)$ OF $k > m$ POINTS IN m-DIMENSION (NOT ALL THE SAME) -k LOCATIONS ON AN m-DIM. OBJECT. k-ADS ARE EQUIVALENT MOD G: A GROUP G OF TRANSFORMATIONS.
- (a). $\Sigma(m, k)$. [KENDALL, 1984, KENT, LE]
- G IS GENERATED BY TRANSLATIONS, SCALING (TO UNIT SIZE), ROTATONS.
- PRESHAPE

$$\mathbf{u} = (x_1 - \langle x \rangle, \ldots, x_k - \langle x \rangle)/\|\mathbf{x} - \langle \mathbf{x} \rangle\|$$

- SHAPE OF k-AD $\sigma(x) \in S^{m(k-1)-1}/SO(m) = \Sigma(m, k)$.

- CASE $m = 2$. PLANAR SHAPES. $M = \Sigma(2, k)$.

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

- $M \simeq S^{2k-3}/S^1 \simeq \mathbb{C}P^{k-2}$ (COMPLEX PROJ. SPACE)
- **EXTRINSIC MEAN** μ_E: EMBEDDING:

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

- G - EQUIVARIANT, $G = SU(k)$: $k \times k$ unitary matrices A ($AA^* = I_k$, $Det(A) = +1$).

$$A\sigma(\mathbf{u}) = A[\mathbf{u}] \equiv [A\mathbf{u}] = \{e^{i\theta}A\mathbf{u} : \; -\pi < \theta \leq \pi\}$$
$$J(A[\mathbf{u}]) = A\mathbf{u}\mathbf{u}^*A^*$$
$$\phi(A) : S(k, \mathbb{C}) \to S(k, \mathbb{C}), \; B \mapsto ABA^*.$$
$$(\phi(A))J([\mathbf{u}]) = \phi(A)(\mathbf{u}\mathbf{u}^*) = A\mathbf{u}\mathbf{u}^*A^*$$

- **PROPOSITION 5.** μ_E EXISTS IFF THE LARGEST EIGENVALUE OF E(UU^*) IS SIMPLE. [$J(\mu_E) = mm^*$, m UNIT EIGENVEC.]
- **INTRINSIC MEAN** μ_I.
- CASE $m > 2$. $\Sigma(m, k)$ HAS SINGULARITIES. ACTION OF $SO(m)$ IS NOT FREE ON M.

(b) REFLECTION-SHAPE SPACE $R\Sigma(m, k)$.

- ASSUME AFFINE SPAN OF EACH k-AD **x** IS $\mathbb{R}^m$, WITH PRESHAPE $\mathbf{u} = (u_1, , u_k) \in S^{m(k-1)-1}$.
- SHAPE $\sigma(x) \in S^{m(k-1)-1}/O(m) = M$. EMBEDDING

$$J : \sigma(x) \mapsto ((u_i \cdot u_j)) \ (M \to S_{0+}(k, R))$$

- **PROPOSITION 6.** LET $\lambda_1 \geq \ldots \geq \lambda_k$ BE EIGENVALUES OF E$((U_i \cdot U_j))$, WITH EIGEN- VECTORS $v_1, \ldots, v_k$, WHERE $|v_j|^2 = \lambda_j/(\lambda_1 + +\lambda_m)$ $(j = 1, \ldots, m)$. (i) μ_E EXISTS IFF $\lambda_m > \lambda_{m+1}$, AND THEN (ii) $J(\mu_E) = (v_1, \ldots, v_m)(v_1, \ldots, v_m)^t$.

(c) AFFINE SHAPE SPACE $A\Sigma(m,k)$, $k > m+1$.

- C(k,m) = k-ADS $u = x - \langle x \rangle$ WITH SPAN $\mathbb{R}^m$
- SHAPE

$$\sigma(x) = \{Au = (Au_1, \dots, Au_k) : \; A \in GL(m,\mathbb{R})\}.$$

- $A\Sigma(m,k) = C(k,m)/GL(m,\mathbb{R})$.
- THE m ROWS OF u LIE IN A HYPERPLANE H OF $\mathbb{R}^k$, $H = \mathbf{1}^\perp \simeq \mathbb{R}^{k-1}$, AND SPAN A SUBSPACE L OF DIM. m OF H. NOW $Au = v$ FOR SOME A IFF THE ROWS OF v SPAN L. HENCE $\sigma(x) \simeq L$.
- THUS $A\Sigma(m,k) \simeq$ GRASSSMANNIAN $G_m(k-1)$. EMBEDDING $J : A\Sigma(m,k) \to S_+(k-1,\mathbb{R})$.

- $\sigma(x) \longrightarrow$ MATRIX OF PROJ. $P_L : H \mapsto L = B^t B$.
- HERE L IS SPANNED BY ORTHONORMAL $w_1, \ldots, w_m$; $w_i = \sum b_{ij} f_j$ ($\{f_1, \ldots, f_{k-1}\}$ ORTH. BASIS OF H); $B = ((b_{ij}))_{1 \leq i \leq m,\ 1 \leq j \leq k-1}$.
- **PROPOSITION 7.** (i) μ_E EXISTS IFF AMONG EIGENVALUES $\lambda_1 \geq \ldots \geq \lambda_{k-1}$ OF THE MEAN OF $B^t B$, $\lambda_m > \lambda_{m+1}$, AND (ii) THEN μ_E IS THE SUBSPACE OF H SPANNED BY THE FIRST m EIGENVECTORS. [CHIKUSE, BP]

(d) PROJECTIVE SHAPE SPACES $P\Sigma(m,k)$, $k > m+1$.

- k-AD $\mathbf{x} = (x_1, \ldots, x_k) \in (R^{m+1})^k$; FOR $x \in R^{m+1}$, $x \neq 0$, DEFINE

  $$[x] = \{\lambda x : \lambda \neq 0\} \text{ (THE LINE THROUGH 0 \& x).}$$

- $$RP^m = \{[x] : \; x \in R^{m+1} \setminus \{0\}\}.$$

- FOR $A \in GL(m+1, R)$, A PROJ. LINEAR TRANSFORMATION α ON RP^m IS

  $$\alpha[x] = [Ax]; \; \alpha \in PGL(m) \text{ [GROUP].}$$

- PROJ. SHAPE OF A k-AD x IS

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

- A k-AD $\{y_1, \ldots, y_k\}$ OF POINTS IN RP^m IS IN *GENERAL POSITION* IF THE LINEAR SPAN OF $\{y_1, \ldots, y_k\}$ IS RP^m.
- THE SPACE OF PROJ. SHAPES OF k-ADS IN GENERAL POSITION IS $P\Sigma(m, k)$.
- A PROJ. FRAME IN RP^m IS AN ORDERED SYSTEM OF $m + 2$ POINTS IN GENERAL POSITION.
- LET I BE AN ORDERED SET OF INDICES $i_1 < i_2 < \ldots < i_{m+2} \leq k$. LET $P_I\Sigma(m, k)$ BE THE SET OF PROJ. SHAPES OF k-ADS x FOR WHICH $\{[x_{i_1}], [x_{i_2}], \ldots, [x_{i_{m+2}}]\}$ IS A PROJ. FRAME.
- GIVEN TWO PROJ. FRAMES $(p_1, \ldots, p_{m+2})$, $(q_1, \ldots, q_{m+2})$, THERE EXISTS A UNIQUE $\alpha \in PGL(m)$ SUCH THAT $\alpha(p_j) = q_j$ FOR ALL j.

- BY ORDERING THE POINTS IN A k-AD SUCH THAT THE FIRST $m+2$ POINTS ARE IN GENERAL POSITION, ONE MAY BRING THIS ORDERED SET, SAY, $(p_1, \ldots, p_{m+2})$ TO THE STANDARD FORM $\{[e_1], \ldots, [e_{m+1}], [e_1 + \ldots + e_{m+1}]\}$ BY A UNIQUE α IN $PGL(m)$.
- THUS MODULO $PGL(m)$, PROJECTIVE SHAPES IN $P_I\Sigma(m.k)$ ARE DISTINGUISHED ONLY BY THE REMAINING $k-m-2$ RP^m-VALUED COORDINATES.
- THUS $P_I\Sigma(m,k) \simeq (RP^m)^{k-m-2}$.
- ONE MAY NOW USE THE V-W EMBEDDING FOR EXTRINSIC ANALYSIS.

4. NONPARAMETRIC TESTS

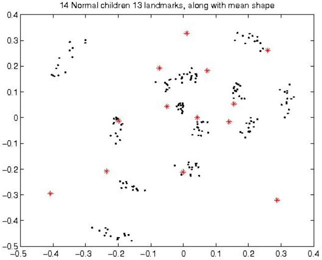
- EMBEDDING $J : M \to E^N$, Q PROB. ON M, Q^J PROB. ON E^N.
- $\mu^J =$ MEAN OF Q^J. (IDENTIFY M WITH $J(M)$)
- $\mu = P\mu^J$ (PROJECTION ON J(M)).
- $\mu_n = P\mu_n^J$ ($\mu_n^J = \frac{1}{n}\sum_{j=1}^n J(X_j)$, X_j iid $\sim Q$).
- COMPUTE ASYMPTOTIC DISTRIBUTION OF $\sqrt{n}(\mu_n - \mu)$ IN THE COORDINATES OF $T_\mu(J(M))$

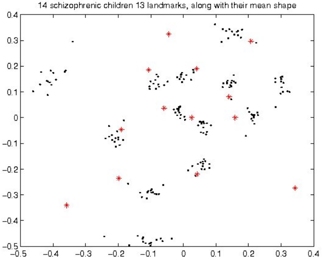
$$\equiv \sqrt{n}(P\mu_n^J - P\mu^J) = \sqrt{n} d_\mu P(\mu_n^J - \mu^J) + o_P(1).$$

TWO SAMPLE PROBLEM: EXAMPLES

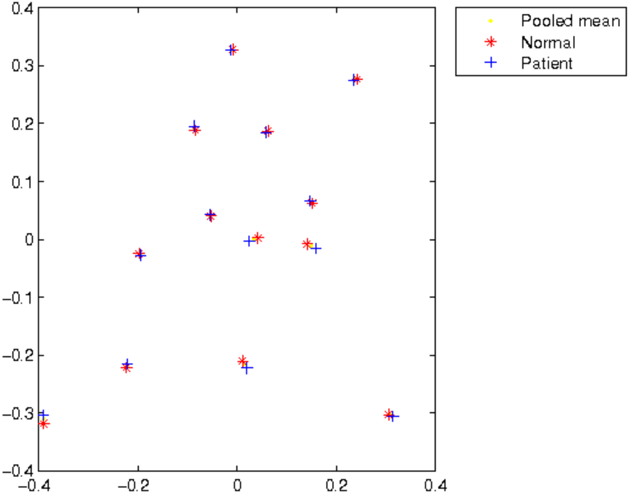
- **1. SCHIZOPHRENIC CHILDREN VS NORMAL CHILDREN** Σ_2^k, $k = 13$. (13 LANDMARKS ON A MIDSAGITTAL 2-D SLICE FROM MR BRAIN SCAN).
- $n = 14, m = 14$
- P-VALUE = 3.8×10^{-11} (EXTRINSIC), 3.97×10^{-11} (INTRINSIC)
- **2. GLAUCOMA DETECTION** (PAIRED SAMPLES). $R\Sigma_3^k$, k=4 (DIM = 5) LANDMARKS ON THE GLAUCOMA INDUCED EYE AND THE NORMAL EYE OF $n = 12$ RHESUS MONKEYS.
- P-VALUE < 0.01 (EXTRINSIC).

SCHIZOPHRENIA PLOTS

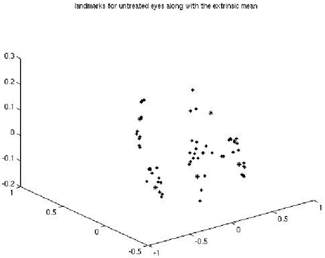


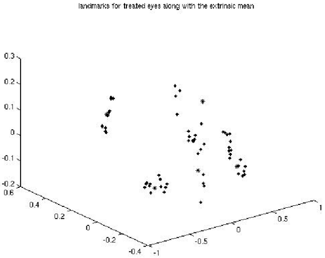


SAMPLE MEAN SHAPES

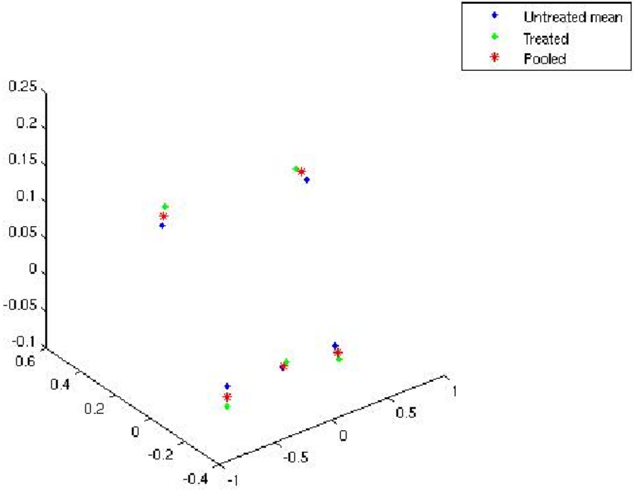


GLUCOMA DETECTION PLOTS





SAMPLE MEAN SHAPES



REFERENCES

- 1. A.Bhattacharya & R.Bhattacharya (2007). *Proc. Amer. Math. Soc.* In Press.
- 2. B & B (2007). *IMS Lecture Ser. In Honor of J.K.Ghosh*. In Press.
- 3. A.Bandulasiri, R.Bhattacharya, & V.Patrangenaru. (2007). *JMVA*, To Appear.
- 4. B & P.(2005). *Ann. Statist.*
- 5. B & P. (2003). *Ann. Statist*.
- 6. K.Mardia & V.Patrangenaru (2005). *Ann. Statist.*
- 7. D.G.Kendall (1984). *Bull. Lond. Math. Soc.*
- 8. D.G.Kendall, D.Barden, T.K.Carne & H.Le(1999). *Shape and Shape Theory*. Wiley.
- 9. J.Kent (1994). *Proc. Royal. Stat. Soc. B.*
- 10. I.Dryden & K.Mardia (1998). Wiley.

- 11. F.Bookstein (1997). Cambridge Univ. Press.
- 12. Y.Chikuse (2003). Springer.
- 13. H.Hendriks and Z.Landsman (1998). JMVA.