K-Sample Test on Compact Manifolds

Hwiyoung Lee

February 24, 2021

Department of Statistics, Florida State University

A Center of Data

Unlike the Euclidean space,

Mean of a distriburion on $\mathcal{M} \neq$ Center of data

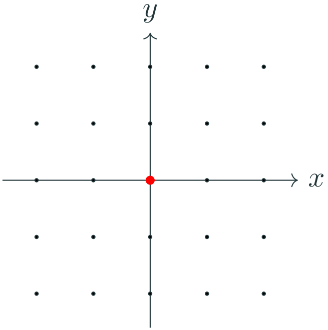


Figure 1: Center of data on $\mathbb{R}^2$ and S^1.

AntiMean

Suppose $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathcal{M}$ consist i.i.d copies of $\mathbf{X}$.

The sample extrinsic antimean :

$$\alpha\overline{\mathbf{X}}_E = J^{-1}\{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})})\}, \text{ where}$$

- Mean vector on ambient Euclidean space :

$$\overline{J(\mathbf{X})} = \frac{1}{n}\sum_{i=1}^{n} J(\mathbf{x}_i)$$

- Farthest Projection : $\mathcal{P}_{\mathsf{F}} : \mathbb{R}^k \to \widetilde{\mathcal{M}}$, s.t for $\forall \mathbf{u}' \in \widetilde{\mathcal{M}}$,

$$\mathcal{P}_{\mathsf{F}}(\mathbf{y}) = \{\mathbf{u} \in \widetilde{\mathcal{M}} : \|\mathbf{u} - \mathbf{y}\| \geqslant \|\mathbf{u}' - \mathbf{y}\|\}$$

Farthest Projection

1. Distinguish two distributions having same extrinsic mean
2. Useful when the extrinsic mean does not exist (or not unique)

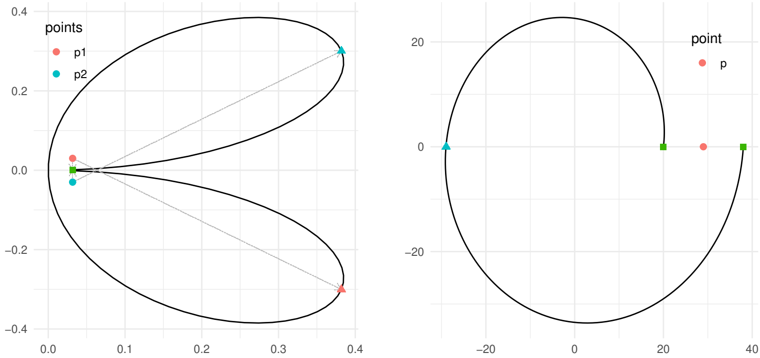


Figure 2: Farthest projection

Weak convergence of the sample Anti Mean

$$\sqrt{n}\left(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}) - \mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu})\right) \xrightarrow{d} N\left(\mathbf{0}_k, \alpha\boldsymbol{\Sigma}_{\boldsymbol{\mu}}\right),$$

$$\alpha\boldsymbol{\Sigma}_{\boldsymbol{\mu}} = \left[\sum_{a=1}^{d} d_{\boldsymbol{\mu}}\mathcal{P}_{\mathsf{F}}(\mathbf{e}_b)\cdot\mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu}))\mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu}))\right]_{b=1,\cdots,k} \boldsymbol{\Sigma}$$
$$\left[\sum_{a=1}^{d} d_{\boldsymbol{\mu}}\mathcal{P}_{\mathsf{F}}(\mathbf{e}_b)\cdot\mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu})\mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu}))\right]_{b=1,\cdots,k}^{\top}$$

$\boldsymbol{\Sigma}$ denotes the covariance matrix of $J(\mathbf{X}_1)$ with respect to the canonical basis $\mathbf{e}_1, \ldots, \mathbf{e}_k$.

Asymptotics of the Sample Anti Mean

- The tangential component of $\mathbf{v} \in \mathbb{R}^k$

$$\tan(\mathbf{v}) = [\mathbf{e}_1(\mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu}))^\top \mathbf{v}, \cdots, \mathbf{e}_d(\mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu}))^\top \mathbf{v}]^\top$$

- The consistent estimator of $\alpha\boldsymbol{\Sigma}_{\boldsymbol{\mu}}$

$$\alpha\mathbf{S}_{E,n} = \left[\sum_{a=1}^{d} d_{\overline{J(\mathbf{X})}}\mathcal{P}_{\mathsf{F}}(\mathbf{e}_b) \cdot \mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}))\mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}))\right]\mathbf{S}_{j,n}$$
$$\left[\sum_{a=1}^{d} d_{\overline{J(\mathbf{X})}}\mathcal{P}_{\mathsf{F}}(\mathbf{e}_b) \cdot \mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}))\mathbf{e}_a(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}))\right]^\top$$

where $\mathbf{S}_{J,n} = \frac{1}{n}\sum_{i=1}^{n}\left(J(\mathbf{X}_i) - \overline{J(\mathbf{X})}\right)\left(J(\mathbf{X}_i) - \overline{J(\mathbf{X})}\right)^\top$

Then we have

$$\sqrt{n}\alpha\mathbf{S}_{E,n}^{-\frac{1}{2}} \tan\left(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}) - \mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu})\right) \xrightarrow{d} N(\mathbf{0}_d, \mathbf{I}_d)$$

Asymptotics of the Sample Anti Mean

And by replacing $\tan(\cdot)$ with $\tan_{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})})}(\cdot)$, s.t.

$$\tan_{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})})}(\mathbf{v}) = [\mathbf{e}_1(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}))^\top \mathbf{v}, \cdots, \mathbf{e}_d(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}))^\top \mathbf{v}]^\top$$

we get

$$\sqrt{n}\alpha \mathbf{S}_{E,n}^{-\frac{1}{2}} \tan_{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})})} \left(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}) - \mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu})\right) \xrightarrow{d} N(\mathbf{0}_d, \mathbf{I}_d)$$

$$n \left\| \alpha \mathbf{S}_{E,n}^{-\frac{1}{2}} \tan_{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})})}(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})}) - \mathcal{P}_{\mathsf{F}}(\boldsymbol{\mu})) \right\|^2 \xrightarrow{d} \chi^2_d$$

K - Sample Test on Compact Manifolds

Notations

- K groups of random samples :

$$\mathcal{D}_1, \cdots, \mathcal{D}_K \overset{\text{indep}}{\sim} \mathcal{Q}_1, \cdots, \mathcal{Q}_K, \text{ where}$$

1. $\mathcal{D}_k = \{\mathbf{X}_k^1, \cdots, \mathbf{X}_k^{n_k}\}$
2. $\{\mathcal{Q}_k\}_{i=1}^K$ are αj-nonfocal probability measure on $\mathcal{M}$

- The whole data set : $\mathcal{D} = \mathcal{D}_1 \cup \cdots \cup \mathcal{D}_K$

Hypothesis Testing for the equality of antimeans :

$$H_0 : \alpha\boldsymbol{\mu}_1 = \cdots = \alpha\boldsymbol{\mu}_K$$
$$H_1 : \alpha\boldsymbol{\mu}_i \neq \alpha\boldsymbol{\mu}_j, \text{ for some } 1 \leqslant i < j \leqslant K.$$

K - Sample Test on Compact Manifolds

The pooled extrinsic antimean :

$$\alpha\boldsymbol{\mu}_E(\boldsymbol{\omega}) = J^{-1}\left(\mathcal{P}_{\mathsf{F}}\left(\omega_1 J(\alpha\boldsymbol{\mu}_1) + \cdots + \omega_K J(\alpha\boldsymbol{\mu}_K)\right)\right), \text{ where}$$

$\boldsymbol{\omega} = (\omega_1, \cdots, \omega_k)$ is the weight imposed on each group.

The pooled sample extrinsic antimean :

$$\alpha\overline{\mathbf{X}}_E = J^{-1}\left(\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{X})})\right), \text{ where}$$

$$\overline{J^{(}\mathbf{X})} = \frac{n_1}{n}J(\alpha\overline{\mathbf{X}}_1) + \cdots + \frac{n_K}{n}J(\alpha\overline{\mathbf{X}}_K).$$

K - Sample Test on Compact Manifolds

Test Statistic and Asympototic distribution

$$T(\mathcal{D}) = \sum_{k=1}^{K} n_k \left\| \alpha \mathbf{S}_k^{-1/2} \tan_{J(\alpha\overline{\mathbf{X}})}(J(\alpha\overline{\mathbf{X}}_k) - J(\alpha\overline{\mathbf{X}})) \right\|^2 \xrightarrow{d} \chi^2_{Kd}$$

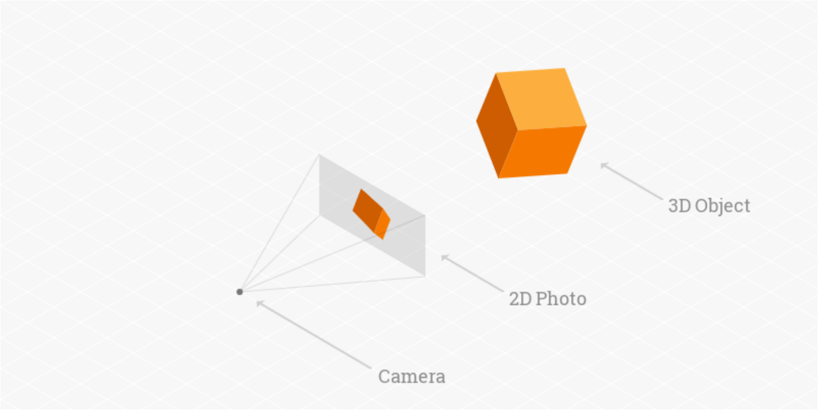
The sample anticovariance matrix of the k th group.

$$\alpha \mathbf{S}_k = \left[\left[\sum_{a=1}^{d} d_{\overline{J(\mathbf{X})}} \mathcal{P}_{\mathsf{F}}(\mathbf{e}_a) \cdot \mathbf{e}_i(J(\alpha\overline{\mathbf{X}}))\mathbf{e}_i(J(\alpha\overline{\mathbf{X}})) \right]_{i=1,\cdots,k} \right] \cdot \mathbf{S}_k$$
$$\left[\left[\sum_{a=1}^{d} d_{\overline{J(\mathbf{X})}} \mathcal{P}_{\mathsf{F}}(\mathbf{e}_a) \cdot \mathbf{e}_i(J(\alpha\overline{\mathbf{X}}))\mathbf{e}_i(J(\alpha\overline{\mathbf{X}})) \right]_{i=1,\cdots,k} \right]^\top$$

where $\mathbf{S}_k = \frac{1}{n_k} \sum_{i=1}^{n_k} \left(J(\mathbf{X}_k^i) - J(\alpha\overline{\mathbf{X}}_k) \right) \left(J(\mathbf{X}_k^i) - J(\alpha\overline{\mathbf{X}}_k) \right)^\top$.

Application to the Projective Shape Space

Graphical Illustration of the Projective Shape



Extrinsic Analysis on $P\Sigma_m^k$

Veronese Whitney Embedding on $\mathbb{R}P^m$

Veronese Whitney Embedding :

$$\begin{aligned} J : \mathbb{R}P^m &\to S_+(m+1, \mathbb{R}) \\ [\mathbf{x}] &\mapsto J([\mathbf{x}]) = \mathbf{x}\mathbf{x}^\top, \end{aligned} \tag{1}$$

where $\mathbf{x} = (\mathbf{x}^1, \cdots, \mathbf{x}^{m+1})^\top \in S^m = \{\mathbf{x} \in \mathbb{R}^{n+1} : \|\mathbf{x}\| = 1\}$.

- The image of the Veronese Whitney embedding

  $J(\mathbb{R}P^m) = \{\mathbf{A} \in S_+(m+1, \mathbb{R}) : \mathrm{rank}(\mathbf{A}) = 1, \mathrm{Trace}(\mathbf{A}) = 1\}$,

- The Veronese Whitney embedding defined on $\mathbb{R}P^m$ is the $SO(m+1) = \{\mathbf{A} \in \mathrm{GL}_{m+1}(\mathbb{R}), \mathbf{A}\mathbf{A}^\top = \mathbf{I}, \det(\mathbf{A}) = 1\}$ equivariant

Anti Mean on $\mathbb{R}P^m$

Suppose $\mathbf{x}_1, \cdots \mathbf{x}_n \in \mathbb{R}P^m$ random objects.

Recall the (sample) extrinsic antimean

$$\alpha\overline{\mathbf{x}}_E = J^{-1}\{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{x})})\},\ \text{where } \overline{J(\mathbf{x})} = \frac{1}{n}J(\mathbf{x}_i)$$

Note : $\overline{J(\mathbf{x})} = \frac{1}{n}J(\mathbf{x}_i)$ belongs to $\mathbf{conv}(J(\mathbb{R}P^m))$

- $\overline{J(\mathbf{x})} \in S_+(m+1, \mathbb{R})$
- $\mathbf{rank}(\overline{J(\mathbf{x})}) \geqslant 1,\ \mathbf{Trace}(\overline{J(\mathbf{x})}) = 1$

Then by SVD

$$\overline{J(\mathbf{x})} = \mathbf{U}\mathbf{D}\mathbf{U}^\top \text{ , where}$$

- $\mathbf{D} = \mathrm{Diag}(\widetilde{\lambda}_{(1)}, \cdots, \widetilde{\lambda}_{(m+1)})$ s.t. $0 \leqslant \widetilde{\lambda}_{(1)} \leqslant \cdots \leqslant \widetilde{\lambda}_{(m+1)}$
- $\mathbf{U} = \left(\widetilde{\gamma}_{(1)}, \cdots, \widetilde{\gamma}_{(m+1)}\right) \in \mathbb{R}^{(m+1)\times(m+1)}$

Now find $\mathcal{P}_{\mathsf{F}}$ of $\overline{J(\mathbf{x})}$ onto $J(\mathbb{R}P^m)$

$$\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{x})}) = \underset{J([\mathbf{p}])\in J(\mathbb{R}P^m)}{\mathrm{argmax}} \|J([\mathbf{p}]) - \overline{J(\mathbf{x})}\|^2$$

Let $\mathbf{U}^\top \mathbf{p} = \mathbf{u} = (u_1, \cdots, u_{m+1})^\top$, and $\|\mathbf{u}\|^2 = 1$

The farthest projection $\mathcal{P}_{\mathsf{F}}$

$$
\begin{aligned}
\|J([\mathbf{p}]) - \overline{J(\mathbf{x})}\|^2 &= \mathrm{Trace}[(\mathbf{p}\mathbf{p}^\top - \overline{J(\mathbf{x})})^2] \\
&= \mathrm{Trace}\left[\left\{\mathbf{U}^\top\left(\mathbf{p}\mathbf{p}^\top - \overline{J(\mathbf{x})}\right)\mathbf{U}\right\}\left\{\mathbf{U}^\top\left(\mathbf{p}\mathbf{p}^\top - \overline{J(\mathbf{x})}\right)\mathbf{U}\right\}\right] \\
&= \mathrm{Trace}\left[(\mathbf{u}\mathbf{u}^\top - \mathbf{D})^2\right] \\
&= \sum_{i=1}^{m+1}(\widetilde{\lambda}_{(i)} - u_i^2)^2 + \sum_{i \neq j}(u_i u_j)^2 \\
&= \sum_{i=1}^{m+1}(\widetilde{\lambda}_{(i)}^2 + u_i^4 - 2\widetilde{\lambda}_{(i)} u_i^2) + \left(\sum_i u_i^2\right)\left(\sum_j u_j^2\right) - \sum_{j=1}^{m+1} u_j^4 \\
&= \sum_{i=1}^{m+1}\widetilde{\lambda}_{(i)}^2 - 2\sum_{i=1}^{m+1}\widetilde{\lambda}_{(i)} u_i^2 + 1 \qquad (*)
\end{aligned}
$$

$(*)$ is maximized when $\mathbf{u} = \mathbf{e}_1 = (1, 0, \cdots, 0)^\top$.

The farthest projection $\mathcal{P}_{\mathsf{F}}$

Since $\mathbf{p} = \mathbf{U}\mathbf{e}_1 = \tilde{\gamma}_{(1)}$

$$\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{x})}) = \mathbf{p}\mathbf{p}^\top = (\mathbf{U}\mathbf{e}_1)(\mathbf{U}\mathbf{e}_1)^\top = \tilde{\gamma}_{(1)}\tilde{\gamma}_{(1)}^\top$$

Thus, the (sample) anti Mean is given by

$$\alpha\overline{\mathbf{x}}_E = J^{-1}\{\mathcal{P}_{\mathsf{F}}(\overline{J(\mathbf{x})})\} = \left[\tilde{\gamma}_{(1)}\right]$$

Veronese Whitney Embedding on $P\Sigma_m^k \simeq (\mathbb{R}P^m)^q$

Suppose we have k-ads with projective frame

$$\mathbf{p} = \left(\boldsymbol{\pi}_1, \cdots, \boldsymbol{\pi}_{m+2}, \mathbf{p}^{\boldsymbol{\pi}}_{m+3}, \cdots, \mathbf{p}^{\boldsymbol{\pi}}_k\right) \in P\Sigma_m^k \simeq (\mathbb{R}P^m)^q$$

Let $\mathbf{y}$ denote the remaining $q = k - m - 2$ points

$$\mathbf{y} = ([\mathbf{x}_1], \cdots, [\mathbf{x}_q])$$

Then the VW embedding J_k of $(\mathbb{R}P^m)^q$ into $S_+(m+1)$

$$\begin{aligned} J_k : \ (\mathbb{R}P^m)^q &\to S_+(m+1, \mathbb{R})^q \\ \mathbf{y} &\mapsto J(\mathbf{y}) = (J([\mathbf{x}_1]), \cdots, J([\mathbf{x}_q])), \text{ where} \end{aligned}$$

J is the VW embedding of $\mathbb{R}P^m$ in (1).

Anti Mean on $P\Sigma_m^k$

A random sample $\mathbf{y}_1, \cdots, \mathbf{y}_n$ from a distribution $\mathcal{Q}$ of $P\Sigma_3^k$, where $\mathbf{y}_i = (\mathbf{y}_i^1, \cdots, \mathbf{y}_i^q)$ and $\mathbf{y}_i^j = [\mathbf{x}_i^j] \in \mathbb{R}P^3, j = 1, \cdots, q$ then the VW sample antimean is given by

$$\alpha \overline{\mathbf{y}}_E = \left(\left[\widetilde{\boldsymbol{\gamma}}_{(1)}^1 \right], \cdots, \left[\widetilde{\boldsymbol{\gamma}}_{(1)}^q \right] \right), \tag{2}$$

where $\left[\widetilde{\boldsymbol{\gamma}}_{(1)}^j \right]$ denotes the unit eigenvector corresponding to the smallest eigenvalue $\tilde{\lambda}_{(1)}^j$ of the matrix $\frac{1}{n} \sum_{i=1}^n [\mathbf{x}_i^j][\mathbf{x}_i^j]^\top$

Test Statistic

Assume $\{\mathbf{Y}_k^i\}_{i=1}^{n_k} \sim \mathcal{Q}_k$ on $(\mathbb{R}P^3)^q$

Test Statistic :

$$T(\mathcal{D}) = \sum_{k=1}^{K} n_k \left[\left(\left[\widetilde{\gamma}^1_{(1)} \right]_{\mathsf{P}} - \left[\widetilde{\gamma}^1_{(1)} \right]_k \right)^\top \widetilde{\mathbf{\Gamma}}_1, \cdots, \left(\left[\widetilde{\gamma}^q_{(1)} \right]_{\mathsf{P}} - \left[\widetilde{\gamma}^q_{(1)} \right]_k \right)^\top \widetilde{\mathbf{\Gamma}}_q \right] \times$$

$$\alpha \mathbf{S}_k^{-1} \left[\left(\left[\widetilde{\gamma}^1_{(1)} \right]_{\mathsf{P}} - \left[\widetilde{\gamma}^1_{(1)} \right]_k \right)^\top \widetilde{\mathbf{\Gamma}}_1, \cdots, \left(\left[\widetilde{\gamma}^q_{(1)} \right]_{\mathsf{P}} - \left[\widetilde{\gamma}^q_{(1)} \right]_k \right)^\top \widetilde{\mathbf{\Gamma}}_q \right]^\top,$$

If $\frac{n_k}{n} \to \omega_k > 0$, as $n \to \infty$, then $T(\mathcal{D}) \xrightarrow{d} \chi^2_{K \cdot 3q}$.

Anti Covariance Matrix

For $s, t = 1, \cdots, q$ and $c, b = 2, 3, 4$,

$$\begin{aligned}\alpha\mathbf{S}_{k(s,c)(t,b)} =& n_k^{-1}(\tilde{\lambda}^s_{(c)} - \tilde{\lambda}^s_{(1)})^{-1}(\tilde{\lambda}^t_{(b)} - \tilde{\lambda}^t_{(1)})^{-1} \times \sum_i^{n_k} \left(\left[\widetilde{\gamma}^s_{(c)}\right]_{\mathsf{P}}^\top [\mathbf{X}_k^i]_s \right) \\ & \left(\left[\widetilde{\gamma}^t_{(b)}\right]_{\mathsf{P}}^\top [\mathbf{X}_k^i]_t \right) \left(\left[\widetilde{\gamma}^s_{(1)}\right]_{\mathsf{P}}^\top [\mathbf{X}_k^i]_s \right) \left(\left[\widetilde{\gamma}^t_{(1)}\right]_{\mathsf{P}}^\top [\mathbf{X}_k^i]_t \right)\end{aligned}$$

$$\begin{pmatrix} \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}_{(1,\cdot),(1,\cdot)} & & & \\ & \ddots & & \\ & & \begin{bmatrix} (2,2) & (2,3) & (2,4) \\ (3,2) & (3,3) & (3,4) \\ (4,2) & (4,3) & (4,4) \end{bmatrix}_{(s,\cdot),(t,\cdot)} & \\ & & & \ddots \end{pmatrix}_{3q\times 3q}$$

Brain landmark data

3D Brain landmark data was collected (Free et al., 2001)

- Landmarks are placed on the surface of a 3D reconstruction of the cortical surface from MRI data
- 24 landmarks located in 58 adult healthy brains of 4 groups
  1. Right-handed Males ($n_1 = 23$)
  2. Left-handed Males ($n_2 = 8$)
  3. Right-handed Females ($n_3 = 20$)
  4. Left-handed Females ($n_4 = 7$)

3D Brain shape data

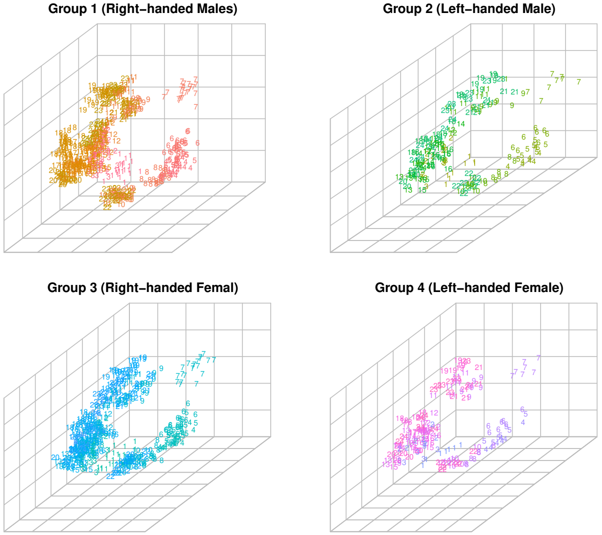


Figure 3: 3D landmarks of Brain shape data.

Results

References

Free, S., O'Higgins, P., Maudgil, D., Dryden, I., Lemieux, L., Fish, D., and Shorvon, S. (2001). Landmark-based morphometrics of the normal adult brain using mri. *NeuroImage*, 13(5):801–813.