Shape Analysis in R

GM library in the light of recent methodological developments

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Outline

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1. **Introduction**
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   - Example 1 – shape data
   - NCS for bivariate data
3. **TPS for shape data**
   - TPS for shape data
   - TPS relaxation along curves
4. **Acknowledgement**

Ian Dryden's R-package — shapes

- **Statistical shape analysis**
- Version: 1.1-3
- `http://www.maths.nott.ac.uk/ ild/shapes`
- Generalized Procrustes Analysis (GPA), Relative Warp Analysis (RWA), statistical inference
- Thin-plate spline grids, 3D visualization via libraries `scatterplot3d` and `rgl`

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- **sliding of semilandmarks on open and closed curves** and surfaces, missing value estimation, affine and non-affine component, unwarping, Multivariate Multiple Linear Regression Model of shape on size, Relative Warp Analysis, shape-space PCA, **form-space PCA**, size-adjusted PCA, 2-block PLS (two shape blocks, one shape block and one block of external variables), analysis of asymmetry, statistical inference
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Introduction

- $x_j \in \mathbb{R}$, k-vector $\mathbf{x}$
- $y_j \in \mathbb{R}$, k-vector $\mathbf{y}$
- $\mathbf{x}_j = \left(x_j^{(1)}, x_j^{(2)}\right)^T \in \mathbb{R}^2$, $k \times 2$ matrix $\mathbf{X}$
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- $f : \mathbb{R} \rightarrow \mathbb{R}$
- $\mathbf{f} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$

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- $f : \mathbb{R} \longrightarrow \mathbb{R}$
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Introduction

- $y_j = f(x_j) + \varepsilon_j$
- $\mathbf{y}_j = \mathbf{f}(\mathbf{x}_j) + \varepsilon_j$

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- **computed tomographies** (CT) of 151 modern humans (78 females and 73 males) of mixed ethnicity, living in France, from birth to adulthood. [Pellegrin Hospital (Bordeaux), Necker Hospital (Paris) and Clinique Pasteur (Toulouse)]

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Data

- each mandibular surface was reconstructed from the CT-scans via the software package **Amira** (Mercury Computer Systems, Chelmsford, MA)
- open-source software **Edgewarp3D** (Bookstein & Green 2002), a 3D-template of 415 landmarks and semilandmarks was created to measure the mandibular surface and was warped onto each mandible

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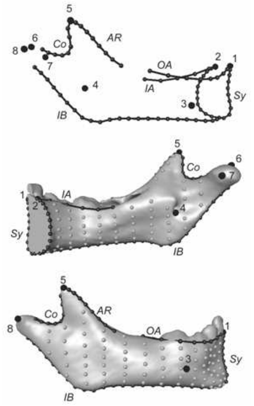

Interpolation model

- Consider a **NCS** given by

$$f(x) = c + ax + \sum_{j=1}^{k} w_j \phi_j(x), j = 1, 2, \ldots k,$$

where

- x_j are the knots, $\phi_j(x) = \phi(x - x_j) = \frac{1}{12}|x - x_j|^3$ with the constraints $\sum_{j=1}^{k} w_j = \sum_{j=1}^{k} w_j x_j = 0$, f'' and f''' are both zero outside the interval $[x_1, x_k]$
- function $\phi(x) = \frac{1}{12}|x|^3$ is a continuous function known as a **radial (nodal) basis function** (Jackson 1989)

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- Let $(\mathbf{S})_{ij} = \phi_j(x_i) = \phi(x_i - x_j) = \frac{1}{12}\left|x_i - x_j\right|^3$, $\mathbf{w} = (w_1, \ldots w_k)^T$
- constraint $(\mathbf{1}_k, \mathbf{x})^T \mathbf{w} = \mathbf{0}$
- **NCS** interpolation to the data (x_j, y_j)

$$\begin{pmatrix} \mathbf{y} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{S} & \mathbf{1}_k & \mathbf{x} \\ \mathbf{1}_k^T & 0 & 0 \\ \mathbf{x}^T & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{w} \\ c \\ a \end{pmatrix}, \quad (1)$$

- where $\mathbf{x}_{k\times1} = (x_1, \ldots x_k)^T$ and $\mathbf{y}_{k\times1} = (y_1, y_2, \ldots y_k)^T$

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Interpolation model

- Let matrix $\mathbf{L}$ be defined as

$$\mathbf{L} = \begin{pmatrix} \mathbf{S} & \mathbf{1}_k & \mathbf{x} \\ \mathbf{1}_k^T & 0 & 0 \\ \mathbf{x}^T & 0 & 0 \end{pmatrix}$$

- inverse of $\mathbf{L}$ is equal to

$$\mathbf{L}^{-1} = \begin{pmatrix} \mathbf{L}_{k \times k}^{11} & \mathbf{L}_{k \times 2}^{12} \\ \mathbf{L}_{2 \times k}^{21} & \mathbf{L}_{2 \times 2}^{22} \end{pmatrix}$$

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- **bending energy matrix** – $k \times k$ matrix $\mathbf{B}_e = \mathbf{L}^{11}$
- constrains of this matrix $\mathbf{1}_k^T \mathbf{B}_e = \mathbf{0}$, $\mathbf{x}^T \mathbf{B}_e = \mathbf{0}$, so the rank of the $\mathbf{B}_e$ is $k - 2$
- $\mathbf{w} = \mathbf{B}_e \mathbf{y}$
- $(c, a)^T = \mathbf{L}^{21} \mathbf{y}$
- $J(f) = \mathbf{w}^T \mathbf{S} \mathbf{w} = \mathbf{y}^T \mathbf{B}_e \mathbf{y}$

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Data pre-processing

- **SVD** of $\mathbf{X}_c = \mathbf{\Gamma}\mathbf{\Lambda}\mathbf{\Gamma}^T = \sum_{j=1}^{2} \lambda_j \gamma_j \gamma_j^T$, $\mathbf{X}_c = \mathbf{X} - \mathbf{1}_k \overline{\mathbf{x}}^T$ (Mardia et al. 2000) [**principal component analysis**]
- the 1th *principal component* of $\mathbf{X}$ is equal to $\mathbf{z}_1 = \mathbf{X}_c \gamma_1$, where γ_1 is the 1th column of $\mathbf{\Gamma}$, and $z_{1j}, j = 1, 2, \ldots k$ are *principal component scores* of jth landmark (z_{1j} is jth element of k-vector $\mathbf{z}_1$)
- re-ordering of the rows of $\mathbf{X}$ is done based on the ranks of z_{1j} in $\mathbf{z}_1$

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- **SVD** of $\mathbf{D}_{dc}$ (Gower 1966) [**principal coordinate analysis**]
- $\mathbf{D}_1$ is $k \times k$ matrix of squared interlandmark Euklidean distances, $\mathbf{D}_2 = -\frac{1}{2}\mathbf{D}_1$ and

$$\mathbf{D}_{dc} = \mathbf{D}_2 - \frac{1}{k}\mathbf{1}_k\mathbf{1}_k^T\mathbf{D}_2 - \frac{1}{k}\mathbf{D}_2\mathbf{1}_k\mathbf{1}_k^T + \frac{1}{k^2}\mathbf{1}_k\mathbf{1}_k^T\mathbf{D}_2\mathbf{1}_k\mathbf{1}_k^T$$

- **doubly centered** (both row- and column-centered)

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Modified interpolation model

- **chordal distance** $d_{ch}^{(j)}$ of the rows $j-1$ and j of $(\mathbf{x}, \mathbf{y})$, $j = 2, 3, ...k$
- **cumulative chordal distance** $d_{cch}^{(j)} = \sum_{i=2}^{j} d_{ch}^{(i)}$, $j = 2, 3, ...k$
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- **chordal distance** $d_{ch}^{(j)}$ of the rows $j-1$ and j of $(\mathbf{x}, \mathbf{y})$, $j = 2, 3, ...k$
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Data

For the purpose of re-sampling

- 21 digitized semilandmarks on the symphisis $\mathbf{X}_{P,2} = (\mathbf{x}_{P,21}, \mathbf{x}_{P,22})$, $\mathbf{d}_{cch,2}$ (subject *No*.2)
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EVAN setting landmarks in science

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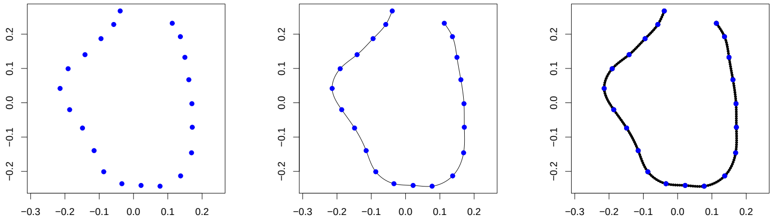

Procrustes shape coordinates, symphisis subject Nr.1 | Procrustes shape coordinates, symphisis subject Nr.1 | Procrustes shape coordinates, symphisis subject Nr.1

Outline

Penalized LRM

- **Penalized linear regression model** (LRM)

$$\mathbf{y}_j = \mathbf{f}\left(\mathbf{x}_j\right) + \varepsilon_j, j = 1, 2, \ldots k,$$

- where $\mathbf{x}_j, \mathbf{y}_j \in \mathbb{R}^2$, $\mathbf{f} = (f_1, f_2) \in \mathcal{D}^{(2)}$ (the class of twice-differentiable, absolutely continuous functions f with square integrable second derivative (Wahba 1990)), $f_m : \mathbb{R}^2 \rightarrow \mathbb{R}, m = 1, 2$
- **penalized sum of squares**

$$S_{pen}\left(\mathbf{f}\right) = \sum_{j=1}^{k} \left\|\mathbf{y}_j - \mathbf{f}(\mathbf{x}_j)\right\|^2 + \lambda J\left(\mathbf{f}\right)$$

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Penalized LRM

- **penalty**

$$J(\mathbf{f}) = \sum_{m=1}^{2} \int \int_{\mathbb{R}^2} \left[\sum_{i,j} \left(\frac{\partial^2 f_m}{\partial x^{(i)} \partial x^{(j)}} \right)^2 \right] dx^{(1)} dx^{(2)}$$

- **penalized least square estimator** $\tilde{\mathbf{f}}$ is defined to be the minimizer of the functional $S_{pen}(\mathbf{f})$ over the class $\mathcal{D}^{(2)}$ of $\mathbf{f}$s, where

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EVAN

Interpolation model

- Consider a **TPS** given by

$$f_m(\mathbf{x}) = c_m + \mathbf{a}_m^T \mathbf{x} + \sum_{j=1}^{k} w_{jm} \phi_j(\mathbf{x})$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{c} + \mathbf{A}^T \mathbf{x} + \mathbf{W}^T \mathbf{s}(\mathbf{x}),$$

where

- $\mathbf{c} = (c_1, c_2)^T$, $\mathbf{A} = (\mathbf{a}_1, \mathbf{a}_2)$, $\mathbf{w}_m = (w_{1m}, w_{2m}, \ldots w_{km})^T$, $m = 1, 2$, $\mathbf{W} = (\mathbf{w}_1, \mathbf{w}_2)$, $\mathbf{s}(\mathbf{x})_{k \times 1} = [\phi_1(\mathbf{x}), \ldots \phi_k(\mathbf{x})]^T$
- function $\phi(\mathbf{x}) = \|\mathbf{x}\|_2^2 \log\left(\|\mathbf{x}\|_2^2\right)$ is a continuous function known as a **radial (nodal) basis function** (Jackson 1989)

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EVAN setting landmarks in science

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- $(\mathbf{S})_{ij} = \phi_j(\mathbf{x}_i) = \phi(\mathbf{x}_i - \mathbf{x}_j),\ i,j = 1,2,\ldots k,\ \forall \|\mathbf{x}\|_2 > 0$
- constraint $\left(\mathbf{1}_k \vdots \mathbf{X}\right)^T \mathbf{W} = \mathbf{0}$
- **TPS** interpolation to the data $(\mathbf{x}_j, \mathbf{y}_j)$

$$\begin{pmatrix} \mathbf{Y} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{S} & \mathbf{1}_k & \mathbf{X} \\ \mathbf{1}_k^T & 0 & \mathbf{0} \\ \mathbf{X}^T & \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{W} \\ \mathbf{c}^T \\ \mathbf{A} \end{pmatrix}, \qquad (2)$$

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Interpolation model

- Let matrix **L** be defined as

$$\mathbf{L} = \begin{pmatrix} \mathbf{S} & \mathbf{1}_k & \mathbf{X} \\ \mathbf{1}_k^T & 0 & \mathbf{0} \\ \mathbf{X}^T & \mathbf{0} & \mathbf{0} \end{pmatrix}$$

- inverse of **L** is equal to

$$\mathbf{L}^{-1} = \begin{pmatrix} \mathbf{L}^{11}_{k\times k} & \mathbf{L}^{12}_{k\times 3} \\ \mathbf{L}^{21}_{3\times k} & \mathbf{L}^{22}_{3\times 3} \end{pmatrix}$$

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Interpolation model

- **bending energy matrix** – $k \times k$ matrix $\mathbf{B}_e = \mathbf{L}^{11}$
- constrains of this matrix $\mathbf{1}_k^T \mathbf{B}_e = \mathbf{0}$, $\mathbf{X}^T \mathbf{B}_e = \mathbf{0}$, so the rank of the $\mathbf{B}_e$ is $k - 2$
- $\mathbf{W} = \mathbf{B}_e \mathbf{Y}$
- $\left(c, \mathbf{A}^T\right)^T = \mathbf{L}^{21} \mathbf{Y}$
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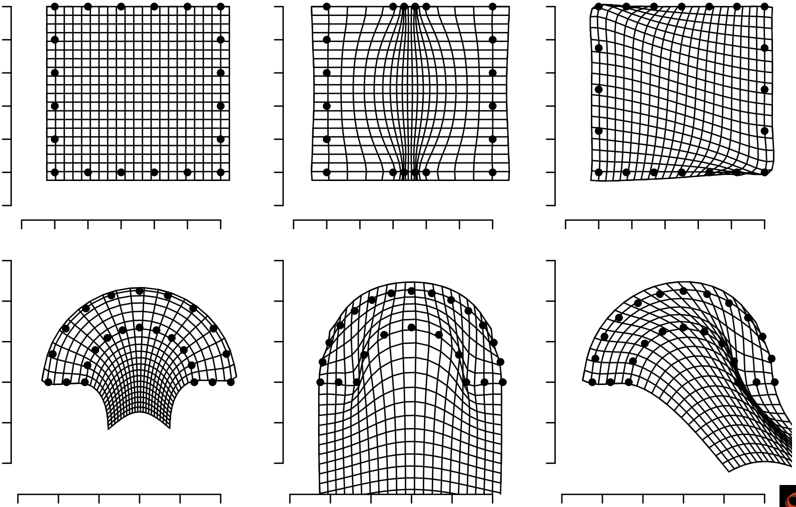

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For the purpose of relaxation

- 21 digitized semilandmarks on the symphisis from subject *No*.2
- its Procrustes shape coordinates $\mathbf{Y} = \mathbf{X}_{P,2}$ were relaxed onto Procrustes shape coordinates $\mathbf{X} = \mathbf{X}_{P,1}$ of subject No.1, seeking the configuration $\mathbf{Y}_r$

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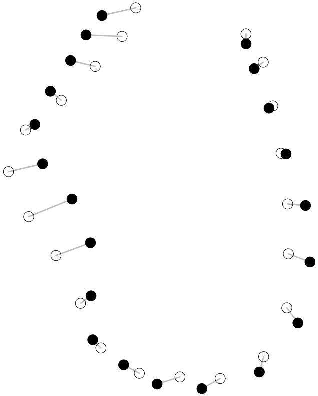

TPS relaxation along curves

- Let $\mathbf{Y}_{k\times 2} = (\mathbf{y}_1, \ldots \mathbf{y}_k)^T$ be configuration matrix with the rows $\mathbf{y}_j = \left(y_j^{(1)}, y_j^{(2)}\right)^T$
- $\mathbf{y}_j^{(r)}$ is free to slid away from their **old position** $\mathbf{y}_j$ along the **tangent directions** $\mathbf{u}_j = \left(u_j^{(1)}, u_j^{(2)}\right)^T$ with $\|\mathbf{u}\|_2 = 1$
- **new position** $\mathbf{y}_j^{(r)} = \mathbf{y}_j + t_j \mathbf{u}_j$
- **tangent directions** $\mathbf{u}_j = \frac{\mathbf{y}_{j+1} - \mathbf{y}_{j-1}}{\|\mathbf{y}_{j+1} - \mathbf{y}_{j-1}\|_2}$
- $\mathbf{U}$ is a matrix of $2k$ rows and k columns in which the (j, j)th entry is $u_j^{(1)}$ and $(k+j, j)$th entry is $u_j^{(2)}$, otherwise zeros

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TPS relaxation along curves

- $\mathbf{y}_r = Vec(\mathbf{Y}_r)$, $\mathbf{B} = diag(\mathbf{B}_e, \mathbf{B}_e)$, $\mathbf{B}_e$ depends only on some configuration $\mathbf{X}$
- $\mathbf{y}_r = \mathbf{y} + \mathbf{Ut}$
- the task is now to minimize the form

$$\mathbf{y}_r^T \mathbf{B} \mathbf{y}_r = (\mathbf{y} + \mathbf{Ut})^T \mathbf{B} (\mathbf{y} + \mathbf{Ut})$$

- setting the gradient of this expression to zero straightforwardly generates the solution (Bookstein 1997)

$$\mathbf{t} = -\left(\mathbf{U}^T \mathbf{B} \mathbf{U}\right)^{-1} \mathbf{U}^T \mathbf{B} \mathbf{y}$$

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TPS relaxation along curves

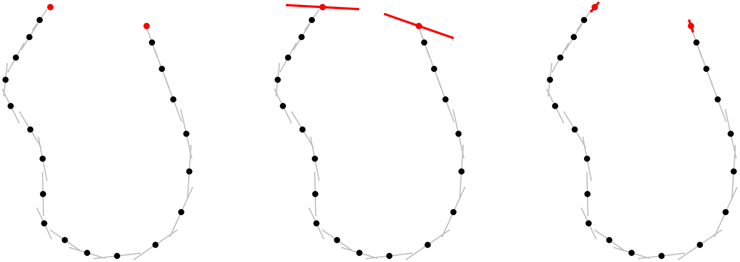
- $\mathbf{y}_r = Vec(\mathbf{Y}_r)$, $\mathbf{B} = diag(\mathbf{B}_e, \mathbf{B}_e)$, $\mathbf{B}_e$ depends only on some configuration $\mathbf{X}$
- $\mathbf{y}_r = \mathbf{y} + \mathbf{Ut}$
- the task is now to minimize the form

$$\mathbf{y}_r^T \mathbf{B} \mathbf{y}_r = (\mathbf{y} + \mathbf{Ut})^T \mathbf{B} (\mathbf{y} + \mathbf{Ut})$$

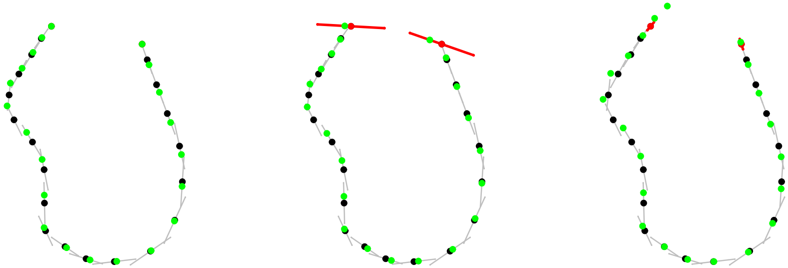
- setting the gradient of this expression to zero straightforwardly generates the solution (Bookstein 1997)

$$\mathbf{t} = -\left(\mathbf{U}^T \mathbf{B} \mathbf{U}\right)^{-1} \mathbf{U}^T \mathbf{B} \mathbf{y}$$

Data



Data



TPS relaxation along curves

- Let the curve defined by $\mathbf{y}_j$ be interpolated by **cubic spline** or **B-spline** $\tilde{f}$ (De Boor (1972) or Eilers & Marx (1996)), $\mathbf{y}_j = (y_j^{(1)}, y_j^{(2)})^T \in \tilde{f}, j = 1, 2, \ldots k$
- **re-sampled points** $\mathbf{y}_i = (y_i^{(1)}, y_i^{(2)})^T \in \tilde{f}, i = 1, 2, \ldots M$ $(M = 500)$ and $\mathbb{M} = \{\mathbf{y}_1, \mathbf{y}_2, \ldots \mathbf{y}_M\}$
- suppose that $\mathbf{y}_j^{(s)} = (y_{sj}^{(1)}, y_{sj}^{(2)})^T \in \tilde{f}$ (the rows of $\mathbf{Y}_S$) are free to slid away from their old position $\mathbf{y}_j$ along the curve $\tilde{f}$

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TPS relaxation along curves

- $J(\mathbf{y}_s) = \mathbf{y}_s^T \mathbf{B} \mathbf{y}_s$, has to be minimized and $\mathbf{y}_r$ is obtained as a minimizer of $J(\mathbf{y}_s)$ given by

$$\mathbf{y}_r = \arg\min_{\mathbf{y}_s} J(\mathbf{y}_s) \tag{3}$$

- the minimization starts with substitution of $\mathbf{y}_1$ by $\mathbf{y}_i \in \mathbb{M}$, ... and ends with substitution of $\mathbf{y}_k$ by $\mathbf{y}_i \in \mathbb{M}$, where $\mathbf{y}_j, j = 1, 2, \ldots k$, are the rows of $\mathbf{Y}$ and $i = 1, 2, \ldots M$:

$$\mathbf{y}_j^{(r)} = \left(\arg\min_{\mathbf{y}_s} J\left(\mathbf{y}_s\right)\right)_{j,k+j}, \tag{4}$$

where $(j, k+j)$th entry of $\mathbf{y}_s$ is substituted by $\mathbf{y}_i^{(s)} \in \mathbb{M}$ for $j = 1, 2, \ldots k; i = 1, 2, \ldots M$, $\mathbf{y}_r = Vec(\mathbf{Y}_r)$ and $\mathbf{y}_j^{(r)}$ are the rows of $\mathbf{Y}_r$

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TPS relaxation along curves

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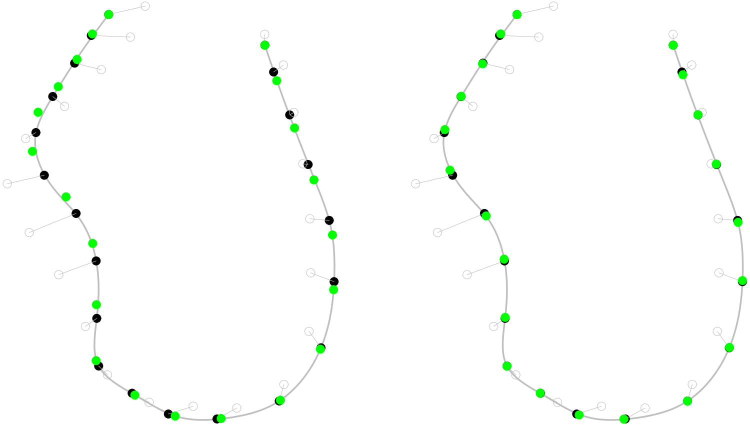
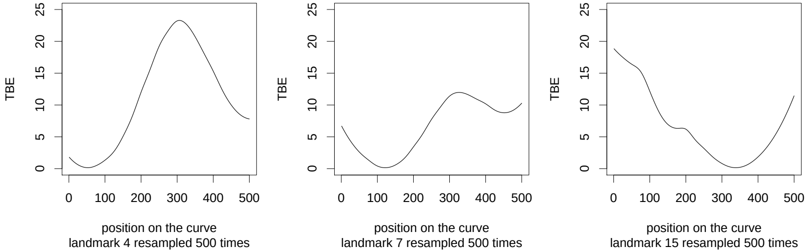
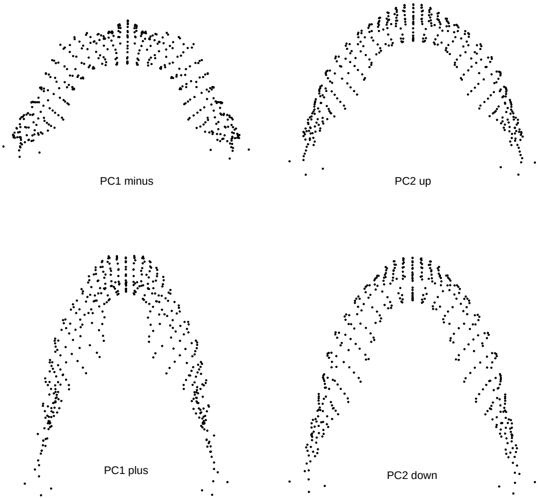


Data


TBE
0
5
10
15
20
25
0
100
200
300
400
500
position on the curve
landmark 4 resampled 500 times
TBE
0
5
10
15
20
25
0
100
200
300
400
500
position on the curve
landmark 7 resampled 500 times
TBE
0
5
10
15
20
25
0
100
200
300
400
500
position on the curve
landmark 15 resampled 500 times

Results of form-space PCA



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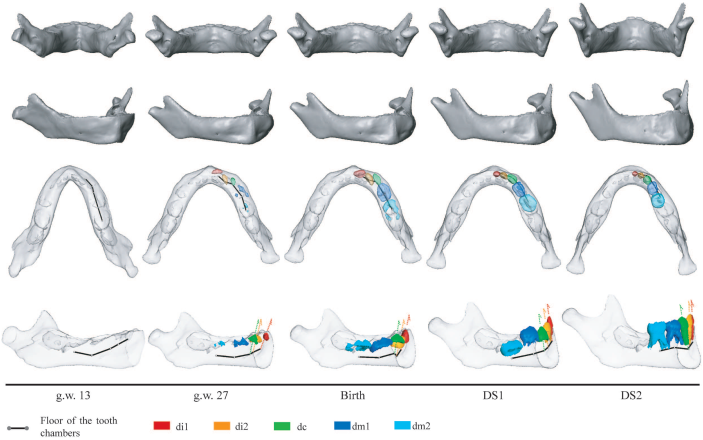

Outline

Acknowledgement

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- **Fred L Bookstein** – University of Vienna, Vienna, Austria and University of Washington, Seattle, US
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