Multivariate Analysis of Data in Curved Shape Spaces

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Outline

1. Landmark analysis
2. Size and shape coordinates
   - The configuration of landmarks
   - Goodall-Mardia coordinates
   - Kendall shape coordinates
3. Statistical analysis of size and shape
   - A quick two-sample test for shape differences
4. References

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Selecting landmarks from an image or object:

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- To reduce the high dimensionality of an image, it is often useful to summarize important features using landmarks.
- Landmark analysis of images is a type of vectorization.
- Salient features of d-dimensional images are encoded as vectors in $\mathbb{R}^{n \times d}$ where n is the number of landmarks.
- Landmarks can be chosen by an expert or by a simple heuristic procedure.

By an expert ....

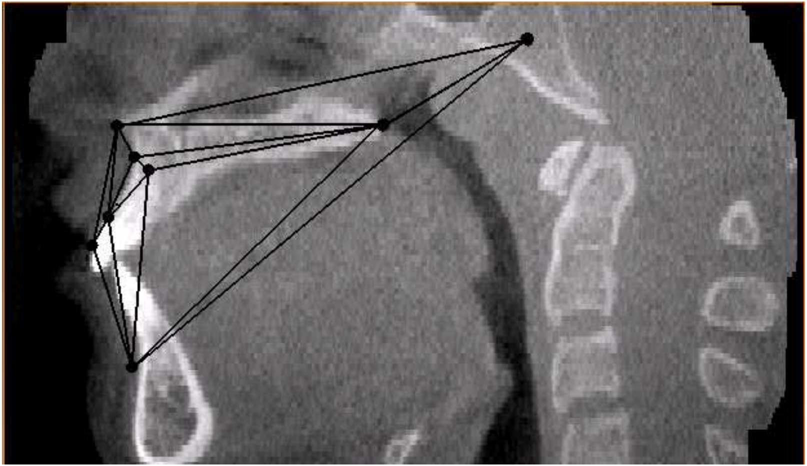

Figure: Seven landmarks from an orthodontics study

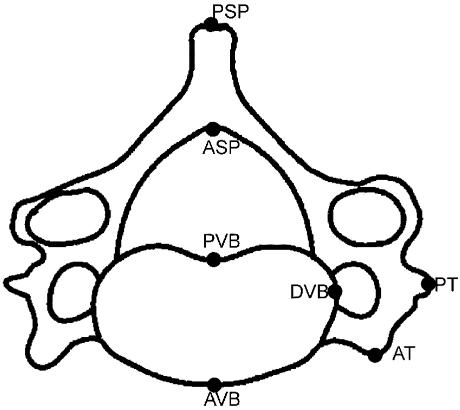

Figure: Landmarks for cervical gorilla vertebra (GGG & GGB)

By a simple heuristic procedure ....

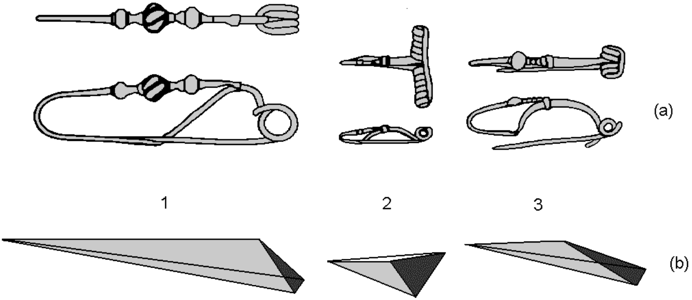

Figure: Iron Age brooch shapes encoded with 4 landmarks

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- to test an hypothesis concerning two or more groups of images.

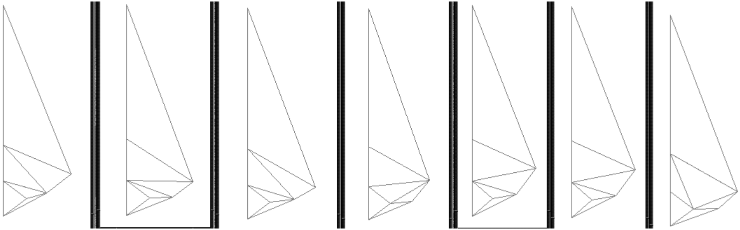
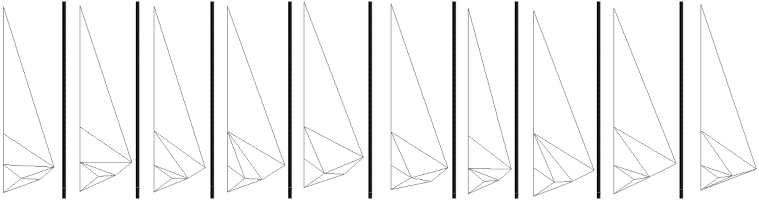


Figure: GGB cervical vertebrae



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Definition

The configuration matrix is defined as

$$X = (X_{ij}), \quad i = 1, \ldots, n; \, j = 1, \ldots, d \, .$$

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Two $n \times d$ configuration matrices

$$(X_{ij}) = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix} \quad \text{and } (Y_{ij}) = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}$$

are said to have the same size and shape if there is some isometry $\tau : \mathbb{R}^d \to \mathbb{R}^d$ such that $Y_i = \tau(X_i)$ for all $i = 1, \ldots, n$.

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- Then $\sim$ defines an equivalence relation on the set of all configuration matrices.
- We write the equivalence class of all configuration matrices Y with the same size and shape as X as $s(X)$.
- Equivalently,

$$s(X) = \{Y \ : \ X \sim Y\}.$$

Outline

Goodall and Mardia (1992), Goodall and Mardia (1993) proposed a representation of the size and shape of landmark cofigurations using lower triangular matrices and the QR-factorization.........

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- We then delete the first row, yielding the $(n-1) \times d$ matrix

$$\widetilde{X} = (X_{ij} - X_{1j}); \quad i = 2, \cdots n; \quad j = 1, \ldots, d\,.$$

called the pre-size-and-shape matrix.

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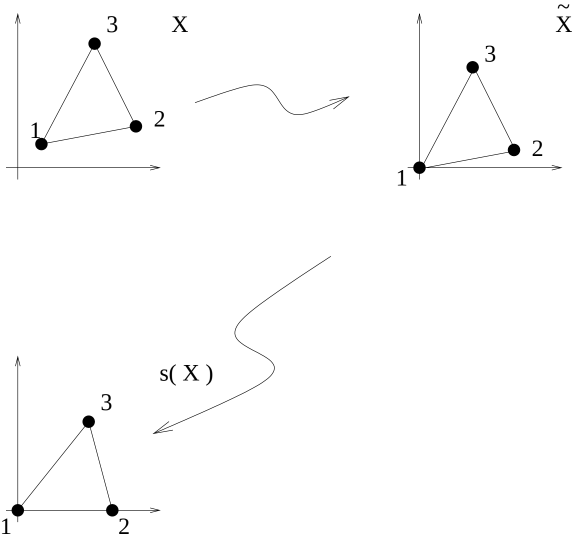
- The matrix $s(X)$ is a coordinate representation of the size and shape of X.

Goodall-Mardia coordinates for size and shape

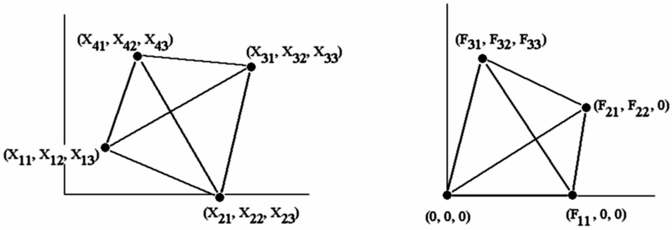
$$s(X) = \begin{pmatrix} F_{11} & 0 & 0 & \cdots & 0 \\ F_{21} & F_{22} & 0 & \cdots & 0 \\ F_{31} & F_{32} & F_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ F_{d1} & F_{d2} & F_{d3} & \cdots & F_{dd} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ F_{(n-1)1} & F_{(n-1)2} & F_{(n-1)3} & \cdots & F_{(n-1)d} \end{pmatrix}$$

where $F_{11}, \ldots, F_{(d-1)(d-1)} > 0$.

For three landmarks in $\mathbb{R}^2$



For four landmarks in $\mathbb{R}^3$



Goodall-Mardia coordinates for shape

To eliminate size, so that only shape information remains, we scale the elements of the size and shape matrix so that $\sigma_{ij} = F_{ij}/F_{11}$. This gives us the shape matrix

$$\sigma(X) = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \sigma_{21} & \sigma_{22} & 0 & \cdots & 0 \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sigma_{d1} & \sigma_{d2} & \sigma_{d3} & \cdots & \sigma_{dd} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sigma_{(n-1)1} & \sigma_{(n-1)2} & \sigma_{(n-1)3} & \cdots & \sigma_{(n-1)d} \end{pmatrix}$$

where again $\sigma_{22}, \ldots, \sigma_{(d-1)(d-1)} > 0$.

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- Goodall-Mardia coordinates provide a simple recipe for representing landmark shapes as multivariate data.
- While the coordinates are represented in lower triangular matrix form, they may be encoded as vectors in standard statistical packages such as R, etc.
- The statistician who wishes to analyse shapes can calculate these coordinates and apply standard multivariate procedures. (While standard distribution assumptions will not hold for the coordinates, they are never realised in practice anyway.)

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- For example, suppose $X^{(1)}, \ldots, X^{(k)}$ are k configurations each of n landmarks in $\mathbb{R}^d$, and let $\pi\left(X^{(1)}\right), \ldots, \pi\left(X^{(k)}\right)$ be row-permuted (i.e., relabelled) versions of the original configurations.

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- Then there is no simple affine relationship between the two sets of shapes

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- A statistician using the former may reach different conclusions from a statistician using the latter.

Outline

In 1986, David G. Kendall proposed a coordinatisation of size and shape based upon procrustes fitting. This is the approach to shape analysis taken in Small (1996, 2011), Dryden and Mardia (1998), Kendall et al. (1999) .....

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- We write size and shape space as

$$S\Sigma_d^n = \left(\Sigma_d^n \times \mathbb{R}^+\right) \cup \{\star\}.$$

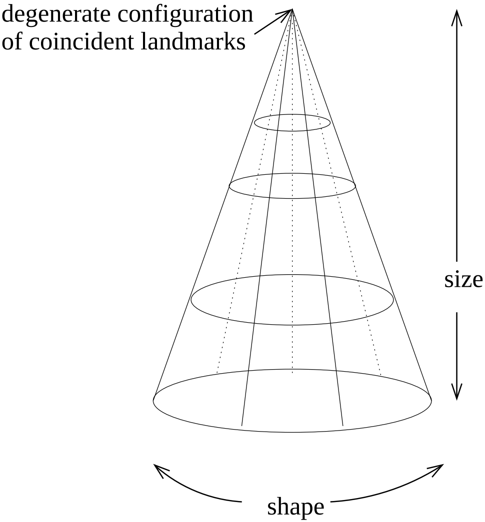

Figure: Schematic diagram of size-and-shape space

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- The shape space Σ_d^n inherits its metric as a subspace of $S\Sigma_d^n$.

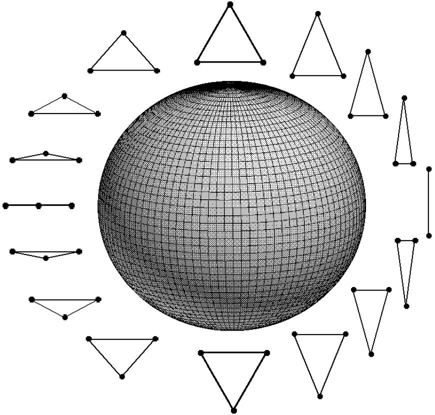
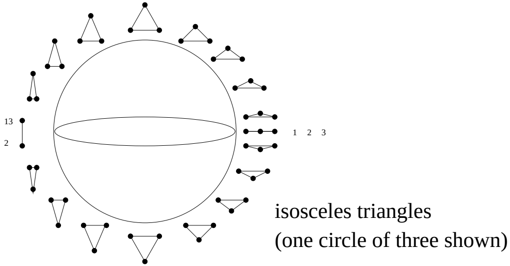


Figure: Shape space Σ_2^3 of triangle shapes in 2D



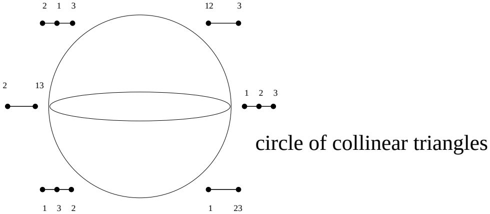


Figure: Shape space Σ_2^3 again. A line of "longitude" corresponding to isosceles triangle shapes (top). The "equator" of collinear triangle shapes (bottom).

Outline

- How do we conduct a statistical analysis of size and shape?

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$$\begin{aligned} \text{Euclidean distance} &\rightarrow \text{Matching distance/Geodesic distance} \\ \text{Centroid} &\rightarrow \text{Frechet mean} \\ \text{MANOVA} &\rightarrow \text{Analysis of geodesic dispersion} \end{aligned}$$

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  - The advantages of this are that the conclusions of such and analysis are not influenced by artificial coordinate systems designed to "make" the data multivariate.
  - The disadvantage of this is that an analog of a multivariate method may not be obviously available, or there may be many different analogs of one multivariate method.

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3. Statistical analysis of size and shape
   - A quick two-sample test for shape differences

4. References

Gorilla gorilla gorilla

Gorilla gorilla beringei

Testing for shape differences in cervical vertebrae of two gorilla subspecies

- We consider the shapes of the fifth cervical vertebrae of two subspecies of gorilla: G. g. gorilla and G. g. beringei.

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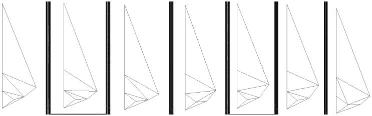

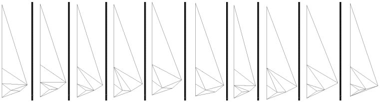

Figure: GGB cervical vertebrae (left), GGG cervical vertebrae (right)

- The most prominent shape differences between the two subspecies are to be seen in the vertex angle at the "top" of the configuration of landmarks: this angle is smaller for GGG than for GGB.
- But is this apparent difference significant? Secondly, which landmarks contribute most to the observed shape differences? Here, we shall only address the first question. See Albert, Le & Small (2003) for more on the second question.

- We test

$$H_0 \; : \; \mathcal{L}\left(\sigma_{GGG}\right) = \mathcal{L}\left(\sigma_{GGB}\right)$$
$$\text{versus}$$
$$H_1 \; : \; \mathcal{L}\left(\sigma_{GGG}\right) \neq \mathcal{L}\left(\sigma_{GGB}\right)$$

where $\sigma \in \Sigma_2^7$ is a random shape from the respective population.

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  where $\sigma \in \Sigma_2^7$ is a random shape from the respective population.

- We shall assume that any differences in shape between GGG and GGB are due to a shift in Frechet mean, and that the geodesic dispersions of the two populations are roughly equal.

- Samples:

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  - GGG: $\sigma_{1,1},\ \sigma_{1,2},\ \ldots,\ \sigma_{1,10}$
  - GGB: $\sigma_{2,1},\ \sigma_{2,2},\ \ldots,\ \sigma_{2,7}$

- Samples:
  - GGG: $\sigma_{1,1}, \sigma_{1,2}, \ldots, \sigma_{1,10}$
  - GGB: $\sigma_{2,1}, \sigma_{2,2}, \ldots, \sigma_{2,7}$

- Proposed test statistic

$$T = \frac{\sum_{j=1}^{10} \sum_{k=1}^{7} \rho^2(\sigma_{1j}\,, \sigma_{2k})}{\sum_{j=1}^{9} \sum_{k=j+1}^{10} \rho^2(\sigma_{1j}\,, \sigma_{1k}) + \sum_{j=1}^{6} \sum_{k=j+1}^{7} \rho^2(\sigma_{2j}\,, \sigma_{2k})}$$

where $\rho(\sigma\,, \tau)$ is the geodesic distance in Σ_2^7 which is the Fubini-Study metric on the complex projective space $\Sigma_2^7 \cong \mathbb{C}P^5(4)$.

- To approximate the distribution of the statistic T under H_0 we can use a permutation test.

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- Shuffle the 10+7=17 shapes into random order:

$$\Pi : \{1, 2, \ldots, 17\} \to \{1, 2, \ldots, 17\},$$

where Π is a random permutation of 1, 2, ... , 17. then partition the shuffled 17 shapes into two new groups:

$$\sigma^*_{1,1}, \ldots, \sigma^*_{1,10}\,; \quad \sigma^*_{2,1}, \ldots, \sigma^*_{2,7}\,.$$

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- We computed the test statistic T^*, iterated 10000 times, and computed the number of times out of 10000 that $T^* > T$.

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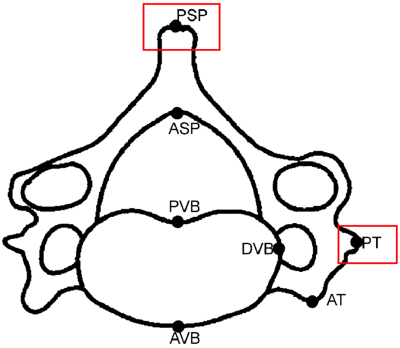
- For the given data, we found only this to be true in only 0.07 % of cases!!!

A more detailed analysis – see Albert, Le & Small (2003) – shows that two landmarks are particularly responsible for most of the between sample shape variation.



Outline

- Albert MH, Le H, Small CG. Assessing landmark influence on shape variation. *Biometrika* 2003, **90**: 669–678.
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Thank you