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Abstract

A growth model for the shape change of biological objects is constructed in terms of a time-varying deformation of the ambient space in which the objects lie. This model is fitted to landmark data using Procrustes tangent coordinates. An example is given based on a set of rat data.

1 Introduction

The purpose of this paper is to construct growth models for the shapes of biological objects in $M = 2$ or 3 dimensions. The basic approach is to construct a time-varying deformation of $\mathbb{R}^M$ which in particular deforms the object of interest. There are three main ingredients in this approach:

(a) a vector space $\mathcal{F}$ of functions in space, $\mathbb{R}^M \to \mathbb{R}^M$, of dimension $p > 0$, say, specifying possible directions of growth;

(b) a vector space $\mathcal{G}$ of functions in time, $\mathbb{R} \to \mathbb{R}$, of dimension $q > 0$, say, specifying possible rates of growth;

(c) a rank r, representing the complexity of the model.

Let $s \in \mathbb{R}^M$ denote a point in the object at time 0, and let t denote (continuous) time. The position of s at time t is modelled by

$$\Phi(s,t) = s + \sum_{l=1}^{r} f_l(s) g_l(t) \tag{1}$$

where $f_l(\cdot) \in \mathcal{F}$, $g_l(\cdot) \in \mathcal{G}$, $l = 1, \ldots, r$. This model is suitable for small levels of growth in which the changes of position can be usefully represented by a linear model. The model can also be extended to allow different growth patterns for different individuals. See e.g. Morris et al. (1999a, 1999b, 2000) for related work.

Two natural choices for $\mathcal{F}$ are based on low order polynomials or on principal warps (Bookstein, 1991, Section 7.5); the latter choice is used here since it gives greater stability near the edges of regions. A natural choice for $\mathcal{G}$ is based on polynomials $g(t)$ satisfying $g(0) = 0$. The choice of the dimensions of these spaces is part of the modelling process.

Since growth is usually dominated by increasing size, it is helpful to look at changes in size and shape separately. For the purposes of this paper we ignore changes in size and limit attention to changes in the shape of the object. Recall that the "shape" of an object comprises all the geometric information about the object except for location, rotation and size (e.g. Dryden and Mardia, 1998). Suppose landmark data are available on different individuals at a common set of ages, taking the form of a 4-way array $\{x_{nkmh}\}$ where

$n = 1, \ldots, N$ labels different individuals, $k = 1, \ldots, K$ labels different landmarks,
$m = 1, \ldots, M$ labels different coordinates, $h = 1, \ldots, H$ labels different times $t_1, \ldots, t_H$.

It is also convenient to represent these data as a collection $\{\boldsymbol{x}_{nh}\}$ of $K \times M$ matrices. In general bold-face will be reserved for $K \times M$ matrices.

2 Procrustes tangent coordinates

Since the shape of an object determines its coordinates only up to a similarity transformation, it is necessary to reduce the model (1) to just the shape information. We do this using Procrustes tangent coordinates about a centered and scaled "mean" configuration $\boldsymbol{\mu}$, say. A convenient choice is the generalized Procrustes estimate based on all NH configurations, but the exact choice does not matter. Let $\boldsymbol{v}_{nh}$ denote the Procrustes tangent coordinates of the data $\boldsymbol{x}_{nh}$. For $f(s) \in \mathcal{F}$, let $f^*(s)$ denote the adjustment of $f(s)$ by adding a linear function of s, so that the $K \times M$ matrix

$$\begin{bmatrix} f(\mu_1)^T \\ \vdots \\ f(\mu_K)^T \end{bmatrix} = f(\boldsymbol{\mu}), \text{ say,}$$

the value of $f(s)$ at the K landmarks in $\boldsymbol{\mu}$, is a Procrustes tangent matrix. Here μ_k denotes the kth row of $\boldsymbol{\mu}$, written as an $M \times 1$ column vector.

Let $\mathcal{F}^*$ denote the vector space of functions $f \in \mathcal{F}$, registered with respect to $\boldsymbol{\mu}$. Let $p^* = \dim(\mathcal{F}^*)$. Note that $p^* \leq p$ since some functions in $\mathcal{F}$ may reduce to the 0 function when adjusted. For example if $M = 2$ and $\mathcal{F}$ contains all linear functions of s (a vector space of dimension 6), then the only linear functions permissible in $\mathcal{F}^*$ are linear combinations of

$$f^*_{0,1}(s) = \begin{bmatrix} s_1 \\ -s_2 \end{bmatrix} \quad \text{and} \quad f^*_{0,2}(s) = \begin{bmatrix} s_2 \\ s_1 \end{bmatrix}. \tag{2}$$

After a suitable approximation and the introduction of an error term, the model (1) takes the form

$$\boldsymbol{v}_{nh} = \boldsymbol{\nu} + \sum_{l=1}^{r} f^*_l(\boldsymbol{\mu})\, g_l(t_h) + \boldsymbol{\epsilon}_{nh}, \tag{3}$$

where $\boldsymbol{\nu}$ is an intercept term. Given orthonormal bases $f^*_{(1)}(s), \ldots, f^*_{(p*)}(s)$ and $g_{(1)}(t), \ldots, g_{(q)}(t)$, the model (3) can also be written in the form

$$\boldsymbol{v}_{nh} = \boldsymbol{\nu} + \sum_{i=1}^{p^*}\sum_{j=1}^{q} a_{ij} f^*_{(i)}(\boldsymbol{\mu}) g_{(j)}(t_h) + \boldsymbol{\epsilon}_{nh} \tag{4}$$

where the matrix of coefficients $A = (a_{ij})$ has rank r.

Assuming an isotropic normal distribution for the errors (which lie in a $2K-4$ dimensional linear space for $M = 2$), maximum likelihood estimation of the parameters A and $\boldsymbol{\nu}$ can be carried out using an alternating algorithm: (a) given A, estimate $\boldsymbol{\nu}$ by averaging suitable residuals from (4) over n and h; and (b) given $\boldsymbol{\nu}$, estimate A using the r dominant components of a singular value decomposition of the $KM \times H$ matrix W, say, where the hth column of W is obtained by summing vec$(\boldsymbol{v}_{nh} - \boldsymbol{\nu})$ over n.

3 Example

We consider a set of rat growth data described and analyzed in Bookstein (1991). The analysis here reinforces his interpretation, but provides a framework for more detailed modelling. The data are obtained from a two-dimensional midsagittal section of the calvarium, (the skull without the lower jaw). There is complete information on $N = 18$ rats at $H = 8$ times (or ages) on $K = 8$ landmarks. To facilitate the model fitting, we replace the actual age by a "pseudo-age" given by the average centroid size at each age, shifted to start at 0 at the initial time.

Consider the model where $\mathcal{F}$ is generated by the linear functions and the dominant two (i.e. coarse scale) principal warps, with $p^* = 4$; where $\mathcal{G} = \text{span}\{t\}$ represents a constant growth rate with $q = 1$; and where the rank is $r = 1$. It can be shown that this model explains the bulk of the variability in the data.

Figure 1 summarizes the fitted model. The Procrustes mean landmarks in $\boldsymbol{\mu}$ are indicated by open circles. The position of the jaw is in the region of the lower right landmark. The growth pattern over the 8 time points is indicated by a straight line at each landmark, blown up by a factor of 2 for visibility, with the initial point indicated by a solid circle. This growth can separated into two spatial components. The linear part can be interpreted as a stretching of the horizontal axis relative to a compression of the vertical axis. The principal warp part can be interpreted roughly

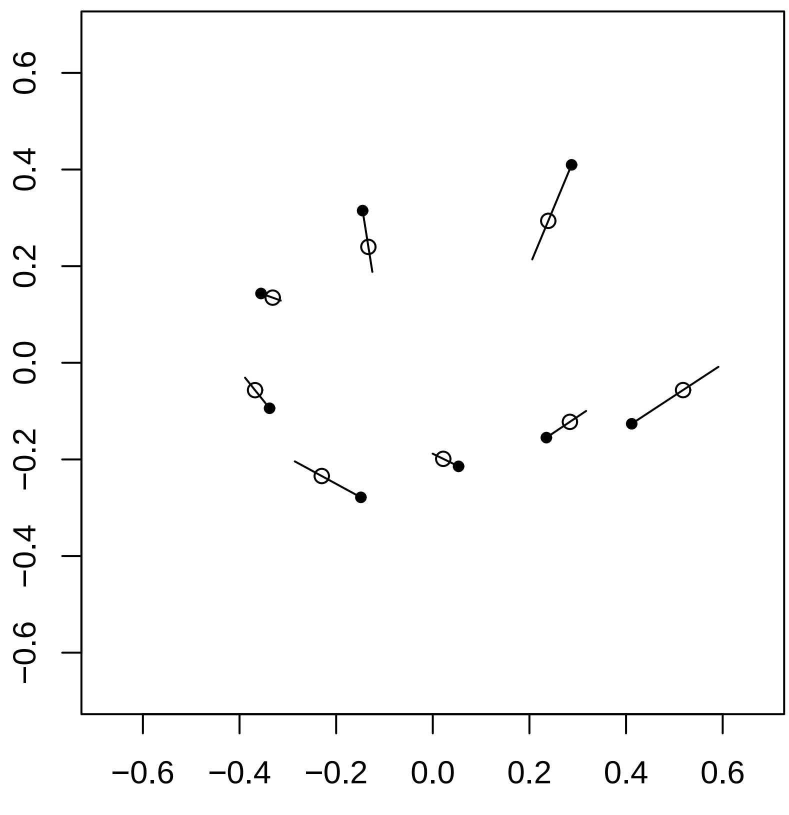

Figure 1: Fitted growth model for the rat data

as a horizontal compression of the top of the skull and a horizontal stretching of the bottom.

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