Curve-fitting in shape spaces

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1 Introduction

The motivation for this work comes from two data sets. The first consists of the three-dimensional coordinates of 62 landmarks on a set of lumbar vertebrae from three primate species (humans, chimpanzees and gorillas). For each animal, measurements were made on five neighbouring vertebrae (L1 - L5). The anatomically significant landmarks were selected by biologists and they felt that 62 landmarks was enough information to capture the essentials of the shapes of the vertebrae. The other data set was first described in Bookstein (1991) and consists of two-dimensional coordinates for eight landmarks on a set of rat skulls. Measurements were made on the rat skulls at various times in the rats' lifetimes (10 days, 20 days, etc.)

The geometric formalism that we use for the mathematical treatment of the shape of objects was established by Kendall in 1984. The shape of an object is defined as 'all the geometrical information that remains when location, scale and rotational effects are filtered out from an object' (Dryden and Mardia, 1998). Given k landmarks in m dimensions, we can construct the shape space , Σ_m^k, in which each point is an orbit of centred, scaled configurations under the action of the group of rotation matrices, $SO(m)$.

What we set out to do is to model shape change, (through either space or time), by fitting curves through sets of points in shape spaces. Shape spaces are non-euclidean and high dimensional, so principal components are used to provide Euclidean tangent projections of the points in shape space for the purposes of visualisation. It is difficult to work in shape space directly, so we fit curves in pre-shape space (where rotation has not yet been quotiented out) and then rotate the pre-shapes of the objects to lie as close to these curves as possible. This is equivalent to working in shape space. In order to establish which curve of a particular type is the best-fitting one, we minimise a sum of squares using the Riemannian metric on shape space, in a way that is analogous to the principles involved in fitting a curve in regression analysis.

We begin by fitting geodesics through sets of points. The principal finding here is that the optimal geodesic through a set of pre-shapes is very close to the geodesic defined by the mean shape of the data set and the first principal component (viewed as a pre-shape). We move on from this to consider non-geodesic curves defined directly on the pre-shape sphere.

Using the orthonormal basis defined by the mean shape and the first two principal components, we can define 'quadratic-type curves' on the pre-shape sphere. The detail of these are included in the main section below. For the rat skull data these quadratic-type curves fit extremely well. For the vertebrae data (which is higher dimensional and seemingly less structured) the curves fit less well, but still better than the geodesics. It is possible to extend the methods described here for more complicated curves. One natural extension is to fit curves based on more principal components than just the first two.

2 Geodesics and quadratic-type curves

Given any pair of orthogonal pre-shapes, v and w, it is possible to define a geodesic, $\Gamma_{(v,w)}$, through that pair of pre-shapes. It can be parametrised by

$$\Gamma_{(v,w)}(s) = (\cos s)v + (\sin s)w \qquad -\frac{\pi}{2} < s < \frac{\pi}{2},$$

where the parameter s is the distance along the geodesic.

Let μ be the mean shape of a set of shapes, and let γ_1 and γ_2 be the first and second principal components respectively. The geodesic $\Gamma_{(\mu,\gamma_1)}$ is our starting point for the construction of a geodesic-type curve. From a point $\Gamma_{(\mu,\gamma_1)}(s)$, we move a distance $t(s)$ along the geodesic defined by this point and γ_2. If $t(s)$ is a quadratic in s then the resultant curve is what we call a 'quadratic-type curve'. Obviously it need not be a quadratic, and freedom of choice of the function $t(s)$ allows us to fit different shapes of curves. If we call the resultant curve $H_{(\mu,\gamma_1,\gamma_2,t)}$ then we have

$$H_{(\mu,\gamma_1,\gamma_2,t)}(s) = (\cos t(s))((\cos s)\mu + (\sin s)\gamma_1) + (\sin t(s))\gamma_2 \qquad -r < s < r,$$

where r is chosen to ensure that the curve H extends beyond all the data points.

A picture of this process is shown in Figure 1 below.

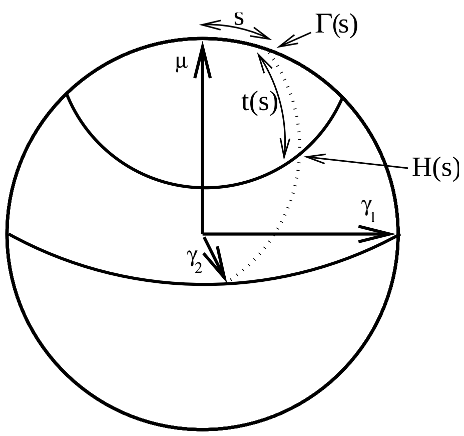

Figure 1: Figure 1: A diagram of a quadratic-type curve

3 Curve-fitting; minimising sums of squares

Suppose we have a data set consisting of n pre-shapes in g groups,

$$\{Z_{11}, Z_{12}, \ldots, Z_{1n_1}, \ldots, Z_{g1}, \ldots, Z_{gn_g}\},$$

and we wish to find the best-fitting quadratic-type curve for the data. For a given quadratic, $t(s) = a_0 + a_1 s + a_2 s^2$, $H_{(\mu,\gamma_1,\gamma_2,t)}$ is a quadratic-type curve. We wish to find a sum of squares associated with H. We could then optimise this sum of squares over the parameters (a_0, a_1, a_2) to find the best-fitting quadratic-type curve.

How far is the pre-shape Z_{ij} from the curve H?

To answer this question we first ask a simpler question. Given a point, $H(s)$ on the curve H, how far is this point from the pre-shape Z_{ij}? Fortunately this question has an easy answer. Using the metric structure of shape space it is possible to define the distance between any two pre-shapes as the shortest great circle distance between the orbits of the two pre-shapes under the action of the group of special orthogonal matrices, $SO(m)$. This Riemannian distance is given the symbol ρ. It is convenient to work with $\sin \rho$, an alternative metric on the space. Thus

$$\sin^2 \rho(Z_{ij}, H(s)) = \min_{R \in SO(m)} \sin^2 \rho(Z_{ij}R, H(s)).$$

To find the distance of the pre-shape Z_{ij} from the curve H, we minimise the function $S = \sin \rho(Z_{ij}, H(s))$ over a suitable range of s.

In our case, when we have more than one pre-shape in each group, we wish to minimise

$$F = \sum_{i=1}^{g} \sum_{j=1}^{n_i} \sin^2 \rho(Z_{ij}, H(\hat{s}_i)),$$

where

$$\hat{s}_i = \operatorname*{argmin}_{-r \leq s \leq r} \sum_{j=1}^{n_i} \sin^2(Z_{ij}, H(s)).$$

The analogy with regression analysis with repeated observations is clear.

4 Results

The first two principal components for the rat data are shown in Figure 2 below with the best-fitting quadratic-type curve.

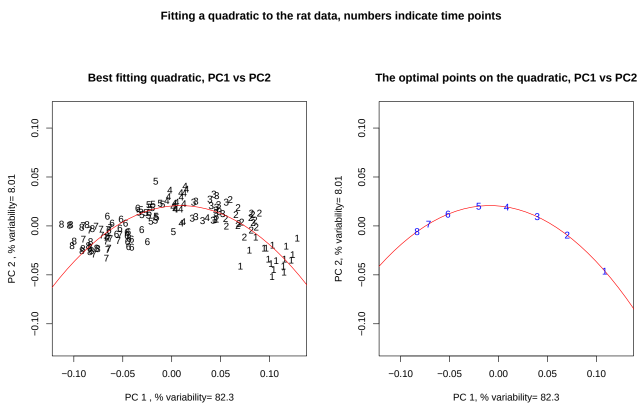

Figure 2: The first two principal components for the rat skull data. Numbers represent time points.

The curve fits the points well and the resultant sum of squares is 0.1091.

When we plot the first two principal components with the best fitting quadratic-type curves for the primate lumbar vertebrae we obtain the plots shown in Figure 3.

Here the fit of the data to the curve is much less convincing. The relevant sums of squares are Chimpanzees 1.3808, Humans 1.1527 and Gorillas 1.3892.

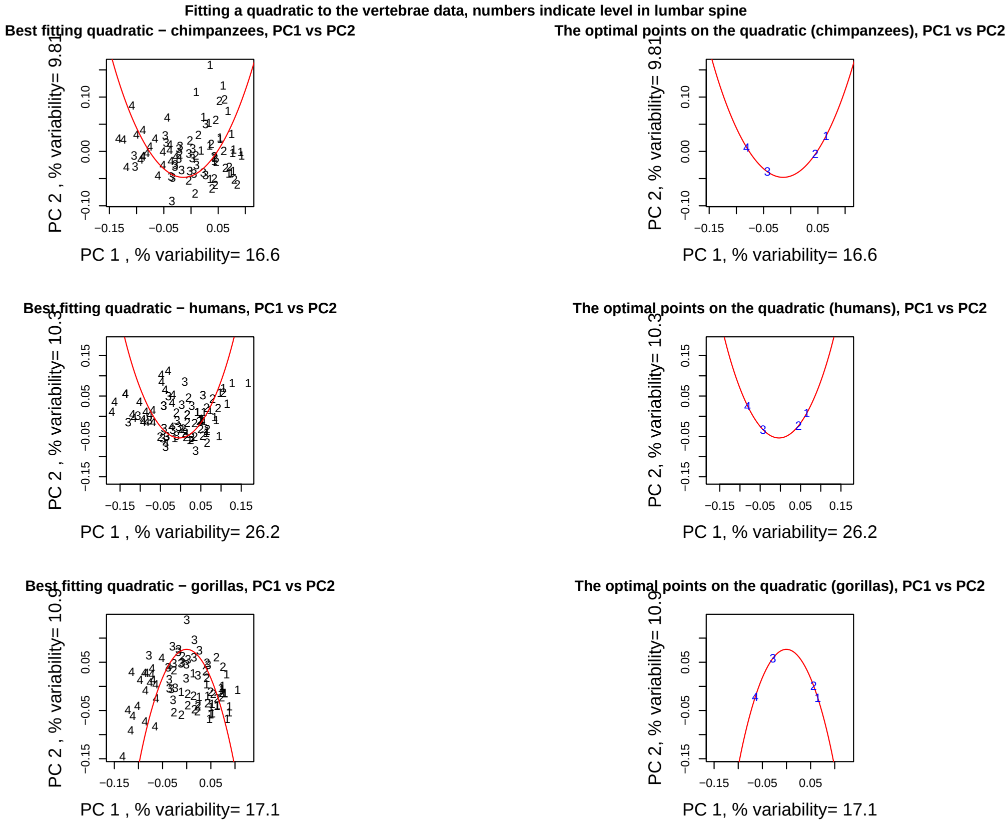

Figure 3: The first two principal components for the primate lumbar vertebrae. Numbers represent levels in spine (L1, L2, etc.)

References

Bookstein, F.L. (1991). *Morphometric Tools for Landmark Data: Geometry and Biology*. Cambridge University Press.

Dryden, I.L. and Mardia, K.V. (1998). *Statistical Shape Analysis*. Wiley, Chichester.

Kendall, D.G.(1984). *Shape manifolds, Procrustean metrics and complex projective spaces*. Bulletin of the London Mathematical Society, 16:81-121.