Curve modeling in shape spaces

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Outline

1. Introduction
2. Shape Curves
3. Shape Splines
4. Discussion
SHAPE

- Geometrical properties that are invariant under certain registration transformations. Some examples...
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- Closed outline shapes: curves which are invariant under diffeomorphic transformations of arc-length.

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- Geometrical properties that are invariant under certain registration transformations. Some examples...
- Euclidean Shape: point sets which invariant under translation, rotation and scale
- Size-and-shape: point sets which invariant under translation and rotation
- Closed outline shapes: curves which are invariant under diffeomorphic transformations of arc-length.
- Note: Quotient spaces often appropriate.
Landmark shapes

- EXAMPLE: Object: $k$ points in $m$ dimensions $X \in \mathbb{R}^{km}$
- Transformation group: Translation, rotation and scale.
- Here there are $k = 50$ points in $m = 2$ dimensions.

- Kendall’s (1984) shape space: $\Sigma_m^k = S^{(k-1)m-1} / SO(m)$.
- Quotient space: Pre-shape sphere with rotation removed.
We wish to register the man ($X_1$) on to the fish ($X_2$), using translation, rotation and scale. $X_1, X_2$ are $k \times m$ matrices, which are centered ($1_k^T X_j = 0$).

Explicit solution: SVD. Procrustes shape distance $d([X_1^P], [X_2])$. 

Practicalities: Procrustes matching
A PRE-SHAPE has had location and scale removed BUT NOT rotation. It lives on a sphere.
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Given two pre-shapes $\mu, z$ the minimal geodesic between their shapes corresponds to

$$\Gamma(s) = \mu \cos s + z \sin s, \quad 0 \leq s \leq \pi/2$$

where $z$ has been Procrustes rotated to $\mu$. 

![Diagram of minimal geodesics on a sphere]
MINIMAL GEODESICS

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  where $z$ has been Procrustes rotated to $\mu$.

Note that this is the horizontal lift of the minimal geodesic in shape space.
EXAMPLE

GEODESIC PATH: Fish $\rightarrow$ Fishman $\rightarrow$ Man

\[ \Gamma(s) = \mu \cos s + z \sin s, \quad 0 \leq s \leq \pi/2. \]
EXAMPLE: RAT SKULLS

Bookstein’s (1991) rat skull data. The rats were carefully X-rayed at age $N$ days, where $N \in \{7, 14, 21, 30, 40, 60, 90, 150\}$.

There are $n = 18$ rats with complete sets of $k = 8$ landmarks at each age in $m = 2$ dimensions.
PCA in tangent space
Minimal geodesic
Joint work with Kim Kenobi and Huiling Le (Nottingham).

Let us consider an extension by introducing another pre-shape $w_2$ which is orthogonal to $w_1$ and $\mu$.

Also, consider a function $t_1(s)$ which gives the position in the direction $w_2$ for each $s$.

The shape curve lifted to the pre-shape space is then defined as:

$$\Gamma_{(\mu, w_1, w_2; t_1)}(s) = \cos\{t_1(s)\} \{(\cos s)\mu + (\sin s)\ w_1\} + \sin\{t_1(s)\}\ w_2,$$
QUADRATIC SHAPE CURVE

\[ t_1(s) = a_0 + a_1 s + a_2 s^2 \]

\[ \Gamma_{(\mu, w_1, w_2; t_1)}(s) = \cos\{t_1(s)\} \{(\cos s)\mu + (\sin s) w_1\} + \sin\{t_1(s)\} w_2, \]
ESTIMATION

Best fitting curve: Minimise

\[ F(a) = \sum_{i=1}^{g} \sum_{j=1}^{n_i} d^2\{[Z_{ij}], \gamma(\hat{s}_i)\} \]

over the parameters \( a \), where \( \hat{s}_i \) minimises

\[ F_{\gamma,i}(s) = \sum_{j=1}^{n_i} d^2\{[Z_{ij}], \gamma(s)\}, \quad i = 1, \ldots, g, \]

and \( \gamma() \) is the shape corresponding to pre-shape \( \Gamma() \), \([Z]\) is the shape of \( Z \), and \( d() \) is a shape distance.
In practice we often have the shapes of $\mu, w_1$ estimated to be almost identical to the Procrustes mean and the first shape PC.

The use of the Procrustes mean and shape PCAs gives an excellent approximation in many applications.

For small $s$ and $t_1(s)$:

$$\Gamma_{(\mu, w_1, w_2; t_1)}(s) \approx \mu + sw_1 + t_1(s)w_2.$$
QUADRATIC-CUBIC SHAPE CURVE

\[ t_1(s) = a_0 + a_1 s + a_2 s^2 \]
\[ t_2(s) = b_0 + b_1 s + b_2 s^2 + b_3 s^3 \]

\[ \Gamma(\mu, w_1, w_2, w_3; t_1, t_2)(s) = \cos\{t_2(s)\} \Gamma(\mu, w_1, w_2; t_1)(s) + \sin\{t_2(s)\} \quad w_3, \]
HYPOTHESIS TESTS

In the quadratic-cubic model there are seven free parameters, \( \{a_0, a_1, a_2, b_0, b_1, b_2, b_3\} \), which specify the curves. We set up three hypotheses which express the different relationships.

- \( H_0: a_0 = a_1 = \ldots = b_3 = 0 \) (Geodesic)
- \( H_1: \) At least one of \( a_0, a_1, a_2 \) is non-zero and \( b_0 = b_1 = b_2 = b_3 = 0 \). (Quadratic)
- \( H_2: \) At least one of \( a_0, a_1, a_2 \) is non-zero and at least one of \( b_0, b_1, b_2, b_3 \) is non-zero. (Quadratic-cubic)
Using a complex Watson model

\[ f([z]) \propto \exp(\kappa \cos^2 d([z], [\mu])), \]

gives the log-likelihoods under the three models as

\[ l_0 = 4766.26, \quad l_1 = 5040.40, \quad l_2 = 5076.82. \]

Thus \(-2(l_0 - l_1) = 548.27, -2(l_1 - l_2) = 72.85\).
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Comparing these statistics with a \(\chi^2_3\) and a \(\chi^2_4\) distribution respectively shows that each reduction in the sum of squares is highly significant.
LIKELIHOOD RATIO TEST

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There is strong evidence against the geodesic and quadratic models in favour of the quadratic-cubic model.
GROWTH ALONG THE QUADRATIC-CUBIC CURVE
ANOTHER EXAMPLE: HOMINIDS

Lumbar vertebra 1-4. Chimpanzee, Gorilla, Human.

$k = 62$ landmarks in $m = 3$ dimensions, $n = 22$ per group.

Data from Paul O’Higgins.
VERTEBRA

Quadratic/quadratic – chimpanzees, PC1 vs PC2

Quadratic/quadratic – gorillas, PC1 vs PC2

Quadratic/quadratic – humans, PC1 vs PC2

Quadratic/quadratic – chimpanzees, PC1 vs PC3

Quadratic/quadratic – gorillas, PC1 vs PC3

Quadratic/quadratic – humans, PC1 vs PC3

PC 1, % variability = 16.6

PC 1, % variability = 17.1

PC 1, % variability = 26.2

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Joint work with Jingyong Su, Anuj Srivastava and Eric Klassen (Florida State) and Huiling Le (Nottingham).

Consider points $p_i$ on manifold $M$ at times $t_i$, $i = 1, \ldots, n$. 

Given Time-Indexed Data

Piecewise-Geodesic Interpolation  Desired Smooth Interpolation
Motivating example

Sequence of outlines of a dancer: 100 points located on outline in 2D.

- Translation, rotation and scale invariance.
- Manifold is Kendall’s shape space (complex projective space).
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- Translation, rotation and scale invariance.
- Manifold is Kendall’s shape space (complex projective space).
- Either: interpolate between data points (here shapes in 2D)
  ![Interpolated shapes]
- Or: smooth a noisy sequence of shapes
Roughness penalty approach

- Find an optimal path $\hat{\gamma}$ by minimizing

$$\frac{\lambda_1}{2} \sum_{i=1}^{n} d(\gamma(t_i), p_i)^2 + \frac{\lambda_2}{2} R(\gamma).$$

- Example roughness penalty: $R(\gamma) = \int_0^1 \left\langle \frac{D^2 \gamma}{dt^2}, \frac{D^2 \gamma}{dt^2} \right\rangle dt$.

Objective function: Data term and Smoothing term.

$$S = \lambda_1 E_d + \lambda_2 E_s.$$  

- Using the Palais metric an explicit expression for the gradient is obtained, leading to a practical fitting algorithm.

- Can use cross-validation to choose $\lambda_2/\lambda_1$. 
Video dancer

Real sequence

Initial path

$\lambda_1 = 0.1, \ \lambda_2 = 1$

$\lambda_1 = 1, \ \lambda_2 = 1$

$\lambda_1 = 100, \ \lambda_2 = 1$
Unrolling and unwrapping splines: Kume et al. (2007)
OTHER APPROACHES

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- Tangent space functional curves: Kent et al. (2001)
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- Tangent space functional curves: Kent et al. (2001)
- Principal nested spheres: Jung et al (2011)
- Local Polynomial Regression: Yuan et al (2011)
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Many other types of non-Euclidean data, high-dimensional, requiring new statistical methodology.
Discussion

- Many other types of non-Euclidean data, high-dimensional, requiring new statistical methodology.

- Statistics/biology/computer science/mathematics/other bridges
Further information


Further information


- Support: EPSRC, Leverhulme Trust, SAMSI

Thank you!
Palais Metric

- Samir et al. (2011) used the Palais metric for computing the gradient of the objective function $S$.
- Let $\gamma$ be a twice differentiable path in manifold $M$ and let $v, w$ be two smooth vector fields along $\gamma$, i.e. $v(t), w(t) \in T_{\gamma(t)}(M)$ for $t \in [0, 1]$. Then, the second-order Palais (1963) metric is:

$$< v(0), w(0) >_{\gamma(0)} + \left< \frac{Dv}{dt}(0), \frac{Dw}{dt}(0) \right>_{\gamma(0)} + \int_{0}^{1} \left< \frac{D^2 v}{dt^2}, \frac{D^2 w}{dt^2} \right>_{\gamma(t)} dt$$

- The explicit form of the gradient is useful for in a practical algorithm for fitting the spline.