Elastic Full Procrustes Means for Sparse and Irregular Planar Curves

Manuel Pfeuffer

Masters Thesis Presentation
Chair of Statistics
Humboldt–Universität zu Berlin

Advisors: Lisa Steyer, Almond Stöcker, Prof. Dr. Sonja Greven

2nd Examiner: Prof. Dr. Nadja Klein

Motivation

Calculate shape means for 2D curves:

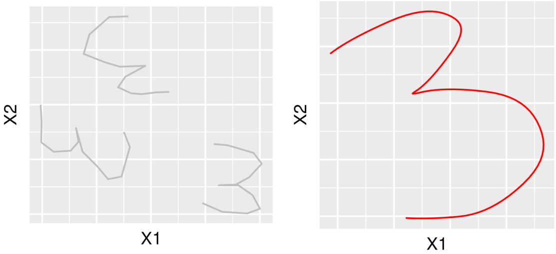

Figure: `digits3.dat` from the `shapes` package (Dryden 2019) with estimated elastic full Procrustes mean. Data: Anderson (1997)

Challenges:

Sparse and irregular, warping, translation/scaling/rotation

Outline

1. What is an Elastic Full Procrustes Mean?
   $\rightarrow$ Sparse and Irregular Planar Curves
   $\rightarrow$ Elastic Mean and Warping
   $\rightarrow$ Full Procrustes Mean and Procrustes Fits
2. Estimation Strategy
   $\rightarrow$ Hermitian Covariance Smoothing
   $\rightarrow$ Estimation of the Procrustes Mean in a Fixed Basis
   $\rightarrow$ Procrustes Fits
3. Results (so far), Problems, Outlook

Sparse and Irregular Planar Curves

How can we compare observations $\beta_i = (\beta_{i1}, \beta_{i2}, \ldots, \beta_{im_i})$?

$\rightarrow$ Treat β_i as functional data $\beta_i(t)$: $\beta_i : [0,1] \rightarrow \mathbb{R}^2$

$\beta_i(t)$ observed at $t_i = (t_{i1}, \ldots, t_{im_i})$:

$$\beta_{i1} = \beta_i(t_{i1}), \ldots, \beta_{im} = \beta_i(t_{im_i})$$

How to find $(t_{i1}, \ldots, t_{im_i})$?

- simple: arc–length
- better: same values of t relate to same "part" of curve

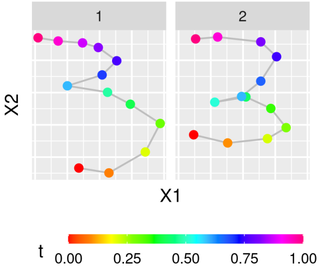

Figure: `digits3.dat` with arc–length parametrisation

Elastic Mean and Warping

Elastic Mean: Mean under optimal re-parametrization (warping).

Well known problem in functional data analysis:

- Perform warping alignment on SRV curves

Square-Root-Velocity (SRV) Framework (Srivasta et al. 2011)

$$q : [0,1] \to \mathbb{R}^2, \quad q(t) = \frac{\dot{\beta}(t)}{\sqrt{||\dot{\beta}(t)||}} \quad \text{for } ||\dot{\beta}(t)|| \neq 0$$

- Use warping methods for sparse and irregular curves as implemented in `elasdics` (Steyer 2021)

Elastic Mean and Warping

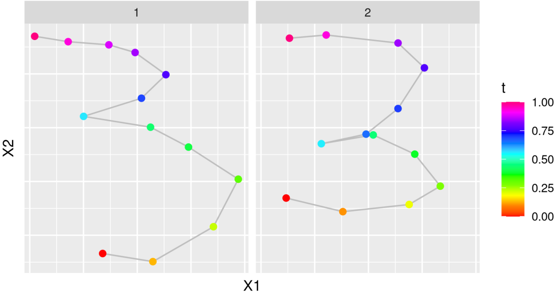

Figure: with `align_curves()` from package `elasdics` (Steyer 2021)

Problem: Methods are not invariant under rotation/scaling!

Full Procrustes Mean and Procrustes Fits

Idea:

1. Calculate SRV mean that is invariant under rotation, scaling
2. Align rotation and scaling of SRV curves to mean
3. Perform warping on aligned SRV curves

Well known problem in **statistical shape analysis** (see e.g. Dryden and Mardia (2016)) $\rightarrow$ 1. Procrustes mean and 2. Procrustes fits

Using complex notation $q_i : [0,1] \rightarrow \mathbb{C}, \quad q_i(t) = x_i(t) + i\, y_i(t)$

we can show that the full Procrustes mean is given by:

$$\mu_q = \underset{z:[0,1]\rightarrow\mathbb{C},\, ||z||=1}{\operatorname{argmax}} \int_0^1 \int_0^1 \overline{z}(s)\, \mathbb{E}\left[\tilde{q}(s)\overline{\tilde{q}}(t)\right] z(t) ds dt$$

with $\tilde{q} = \frac{q}{||q||}$ a random, normalized SRV curves.

Full Procrustes Mean and Procrustes Fits

Population level full Procrustes mean:

$$\mu_q = \underset{z:[0,1]\to\mathbb{C},\, ||z||=1}{\operatorname{argmax}} \int_0^1 \int_0^1 \overline{z}(s) C(s,t) z(t) ds dt$$

- $\rightarrow$ $\mathbb{E}\left[\tilde{q}_i(s)\overline{\tilde{q}}_i(t)\right]$ is the complex covariance function $C(s,t)$
- $\rightarrow$ Functional PCA problem (see Ramsay and Silverman (2005))
- $\rightarrow$ Solution is the leading complex eigenfunction of $C(s,t)$
- $\rightarrow$ We only need to find a good estimate $\hat{C}(s,t)$ to get $\hat{\mu}_q$!

Procrustes fits:

$$\hat{q}_i^P = \langle \tilde{q}_i, \hat{\mu}_q \rangle \tilde{q}_i$$

Reminder: $\cos(\theta) = \langle \vec{x}, \vec{y} \rangle$

Hermitian Covariance Smoothing

Treat estimation of $C(s,t) = \mathbb{E}[\tilde{q}(s)\overline{\tilde{q}}(t)]$ as a regression problem:

- non-parametric regression: $\mathbb{E}[y] = f(s,t)$
- treat parametrisation t_{ij}, t_{ik} as "covariates" s and t
- we can build response $y_{ijk} = \tilde{q}_i(t_{ij})\overline{\tilde{q}}_i(t_{ik})$
- use $\hat{C}(s,t) = \hat{f}(s,t)$ for functional PCA

Note: Using symmetry properties of $C(s,t)$ is important for efficient estimation (see Cederbaum, Scheipl, and Greven (2018)).

$\rightarrow$ use every combination (t_{ij}, t_{ik}) only once

Hermitian Covariance Smoothing

Here: Complex covariance function is hermitian $C(s,t) = \overline{C}(t,s)$

$$\mathbb{E}[Re(y)] = f_{symm}(s,t)$$

$$\mathbb{E}[Im(y)] = f_{skew}(s,t)$$

- model real and imaginary parts seperately
- use `mgcv` (Wood 2017) with symmetric and skew-symmetric tensor product P-splines from `sparseFLMM` (Cederbaum, Volkmann, and Stöcker 2021)

We get:

$$\hat{C}(s,t) = b(s)^T \hat{\Xi} b(t), \quad \text{with} \quad \hat{\Xi} = \hat{\Xi}_{symm} + i\,\hat{\Xi}_{skew}$$

Hermitian Covariance Smoothing

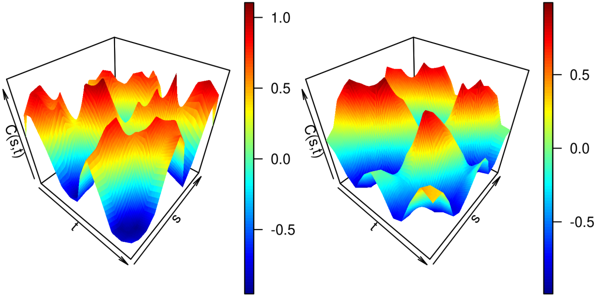

Figure: Estimated real (left) and imaginary (right) parts of $C(s,t)$

Empirical Procrustes Mean in a Fixed Basis

Idea: Estimate covariance function and mean in the same basis:

$$\hat{\mu}_q(t) = b(t)^T \hat{\theta}_\mu$$

Then we can solve the optimization problem directly on $\hat{\Xi}$:

$$\hat{\theta}_\mu = \underset{\theta:\theta^H G\theta = 1}{\operatorname{argmax}} \; \theta^H G \hat{\Xi} G \theta \quad \text{with} \quad G_{kl} = \langle b_k, b_l \rangle$$

$\Rightarrow$ Solution is the leading normalized eigenvector of $\hat{\Xi} G$

Procrustes Fits

Using $\hat{\mu}_q(t) = b(t)^T \hat{\theta}_q$ we can estimate the Procrustes fits:

$$\hat{q}_i^P = \langle \tilde{q}_i, \hat{\mu}_q \rangle \tilde{q}_i$$

- at the moment: integration with linear interpolation of $\tilde{q}_i$'s
- alternative: smoothing in mean basis with $\langle \hat{\tilde{q}}_i, \hat{\mu}_q \rangle = \hat{\theta}_i^H G \hat{\theta}_\mu$

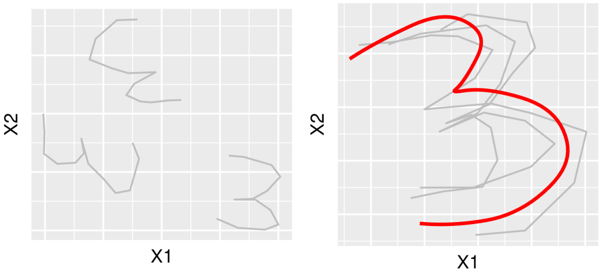

Figure: Procrustes fits and mean (on full dataset) before warping.

Putting it all together

Algorithm Elastic Full Procrustes Mean

Input: Data curves $\beta_1, \dots, \beta_N$
Output: Procrustes mean $\hat{\mu}$ and Procrustes fits $\hat{\beta}_1^P, \dots, \hat{\beta}_N^P$

initialize arc–length parametrisation t_i for all β_i
calculate normalized SRV curves $\tilde{q}_i = \frac{q_i}{||q_i||}$
while convergence not reached **do**
    estimate $C(s, t)$ using t_i
    calculate $\hat{\mu}_q$ as the leading eigenfunction of $\hat{C}(s, t)$
    estimate Procrustes fits $\tilde{q}_i^P$
    update $t_i \leftarrow t_i^{optim}$ using warping alignment on $\hat{\tilde{q}}_i^P$
end while
return integrated Procrustes mean and fits

Results

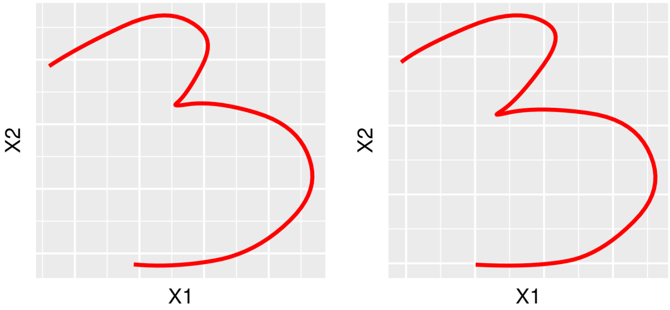

Figure: Full Procrustes mean (left) and elastic full Procrustes mean (right) on `digits3.dat` with with piecewise linear splines on SRV level.

Results / Problems

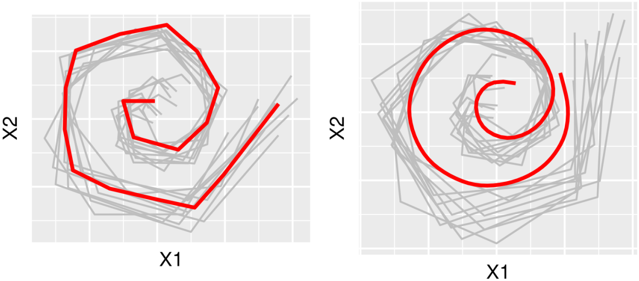

Figure: Elastic full Procrustes mean and procrustes fits for piecewise constant (left) and piecewise linear (right) splines on SRV level.

→ Consistent results only for piecewise constant splines and zero order penalty.

Problems

Normalization: $\tilde{q}_i = \frac{q_i}{||q_i||}$ is itself an estimate ($||q_i|| = \sqrt{\langle q_i, q_i \rangle}$)

$\rightarrow$ can either restrict β_i's to unit–length or normalize q_i directly

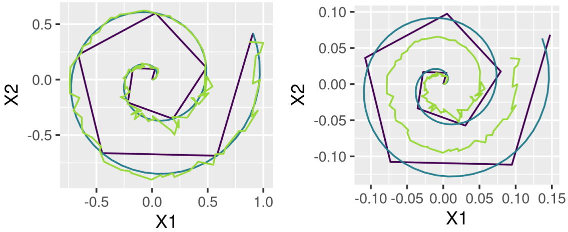

Figure: Spirals (left) and unit–length spirals (right).

$\rightarrow$ likely need smoothing (in the mean basis?) for this

$\rightarrow$ only ok, as long as all curves have same "amount" of sparsity

Outlook

Next steps:

- Real world data application (open curves)
- Better normalization / estimation of procrustes fits

Nice to have (maybe later):

- Mean for closed curves
- Real world data application (closed curves)
- **Code**: bugs, testcases, package, faster

Timeline: Would like to be finished by July

References

- Anderson, C. R. (1997). *Object recognition using statistical shape analysis*. PhD thesis. University of Leeds.
- Cederbaum, J., F. Scheipl, and S. Greven (2018). "Fast symmetric additive covariance smoothing". In: *Computational Statistics & Data Analysis* 120, pp. 25–41.
- Cederbaum, J., A. Volkmann, and A. Stöcker (2021). *sparseFLMM: Functional Linear Mixed Models for Irregularly or Sparsely Sampled Data*. R package version 0.4.0. URL: https://CRAN.R-project.org/package=sparseFLMM.
- Dryden, I. L. (2019). *`shapes` package*. Contributed package, Version 1.2.5. R Foundation for Statistical Computing. Vienna, Austria. URL: http://www.R-project.org.

- Dryden, I. L. and K. V. Mardia (2016). *Statistical shape analysis. With applications in R*. Vol. 995. John Wiley & Sons.
- Ramsay, J. and B. W. Silverman (2005). *Functional Data Analysis*. Springer series in statistics.
- Srivasta, A. et al. (2011). "Shape analysis of elastic curves in euclidean spaces". In: *IEEE Transactions on Pattern Analysis and Machine Intelligence* 33.7, pp. 1415–1428.
- Steyer, L. (2021). *elasdics: Elastic Analysis of Sparse, Dense and Irregular Curves*. R package version 0.1.1. URL: https://CRAN.R-project.org/package=elasdics.
- Steyer, L., A. Stöcker, and S. Greven (2021). "Elastic analysis of irregularly or sparsely sampled curves". In: Preprint.
- Wood, S.N (2017). *Generalized Additive Models: An Introduction with R*. 2nd ed. Chapman and Hall/CRC.

Derivation: Empirical Full Procrustes Mean