ESTIMATING A COVARIANCE FUNCTION FROM FRAGMENTS OF FUNCTIONAL DATA

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FUNCTIONAL DATA: USUAL SETTING

• In statistics, we are often interested in a random variable *X* observed for *n* individuals (e.g. salary, blood pressure, age).

• Here *X* is a random function:

for each of *n* individuals, we observe an entire curve X(t), $t \in \mathcal{I}$, where \mathcal{I} is a compact interval.

• We observe *n* i.i.d. functions $X_1, \ldots, X_n \sim X$.

EXAMPLE: GROWTH CURVES

Growth curves of 39 boys and 54 girls between age 1 and 18. $X_i(t)$: height of *i*th child at age $t \in \mathcal{I} = [1, 18]$



EXAMPLE: RAINFALL CURVES

Rainfall curves from 43 northern and 147 southern Australian weather stations. $X_i(t)$: rainfall at *i*th station at time $t \in \mathcal{I} = [1, 365]$



MEAN AND COVARIANCE

• The mean μ of *X* is a function defined on the interval \mathcal{I} by

 $\mu(t) = E[X(t)], \text{ for each } t \in \mathcal{I}.$

• The covariance function of *X* is a function K(s,t) of *s* and *t* in \mathcal{I} , defined by

$$K(s,t) = \operatorname{cov}\{X(s), X(t)\} = E\Big([X(s) - E\{X(s)\}] [X(t) - E\{X(t)\}] \Big).$$

It describes the variability of the population.

EIGENFUNCTIONS

• Let ϕ_1, ϕ_2, \ldots be orthogonal eigen fct. with resp eigen val. $\theta_1 \ge \theta_2 \ge \ldots \ge 0$ of the operator

$$\psi \in L^2(\mathcal{I}) \longrightarrow \int_{\mathcal{I}} K(s,t)\psi(t) \, dt$$
.

• That is:

$$\int_{\mathcal{I}} K(s,t)\phi_j(s)\,ds = \theta_j\phi_j(t)\,.$$

• Under mild assumptions (Mercer's theorem), can decompose *K* into

$$K(s,t) = \sum_{j=1}^{\infty} \theta_j \,\phi_j(s) \,\phi_j(t) \,,$$

where converence is uniform over s and $t \in \mathcal{I}$.

IN PRACTICE

• In practice, using the observed X_1, \ldots, X_n , we estimate $\mu(t)$ and K(s, t) by

$$\hat{\mu}(t) = \bar{X}(t) = \frac{1}{n} \sum_{i=1}^{n} X_i(t)$$
$$\hat{K}(s,t) = \frac{1}{n} \sum_{i=1}^{n} \{X_i(s) - \bar{X}(s)\} \{X_i(t) - \bar{X}(t)\}.$$

• ϕ_j 's and θ_j 's can be estimated empirically from the data (requires discretising integrals).

EXAMPLE: RAINFALL CURVES

Rainfall curves from 43 northern and 147 southern Australian weather stations. $X_i(t)$: rainfall at time $t \in \mathcal{I} = [1, 365]$



The first four eigenfunctions for the Australian rainfall data explain 70.4%, 24.8%, 3% and 1% of the variability of X:



DIMENSION REDUCTION

• The functions X_i can be written as

$$X_i(t) = \mu(t) + \sum_{j=1}^{\infty} \alpha_{ij} \phi_j(t).$$

• The ϕ_j 's are such that the first few are the most important:

$$X_i(t) \approx \mu(t) + \sum_{j=1}^p \alpha_{ij} \phi_j(t).$$

Example: Rainfall data approximated by the first \boldsymbol{p} terms







FUNCTIONAL DATA OBSERVED IN THE FORM OF FRAGMENTS

- We are interested in curves X_1, \ldots, X_n defined on a compact interval $\mathcal{I} = [a, b]$.
- But: X_j observed only on a compact set $\mathcal{I}_j = [A_j, B_j] \subseteq \mathcal{I}_0$.
- Thus observe one or several fragments of curves.

FRAGMENTS – EXAMPLE: GROWTH DATA



partially observed growth curves of 43 females.

Problem

- Goal: estimate covariance function K(s,t) for all $s, t \in \mathcal{I}$.
- Can compute the empirical covariance estimator only for |s t| small:

$$\hat{K}(s,t) = \frac{1}{n} \sum_{i=1}^{n} \{X_i(s) - \bar{X}(s)\} \{X_i(t) - \bar{X}(t)\}$$

• $\hat{K}(s,t)$ requires to observe $X_i(s)$ and $X_i(t)$ and we only have that for |s-t| small.



A COVARIANCE FUNCTION



Covariance function Cov(X(s), X(t)) to estimate.

WHERE WE OBSERVE DATA



Scatterplot of points (s, t) at which at least one of n = 100 such partial curves was observed.

SPARSE VERSUS FRAGMENTS

- Methods exist for "sparse functional data"; see Yao, Müller and Wang (2005).
- They assume *i*th curve is observed at a small number of points T_{ij} , where $j = 1, ..., N_j$.
- They assume the T_{ij} 's are i.i.d.
- Not designed for data in the form of fragments.

Sparse versus fragments



Left: sparse data. Right: fragments of curves.

ILLUSTRATION OF WHY SUCH METHODS FAIL FOR FRAGMENTS



Covariance function Cov(X(s), X(t)) to estimate.

ILLUSTRATION OF WHY SUCH METHODS FAIL FOR FRAGMENTS



Scatterplot of points (s, t) at which at least one of n = 100 partial curve was observed.

METHOD DESIGNED FOR FRAGMENTS

- Data are poor: cannot use sophisticated or consistent nonparam methods.
- In Delaigle and Hall (2013) we suggested a first very simple method.
- Very basic: based on copying and pasting vertically shifted fragments to each fragment.
- Then essentially use the extended fragments for inference.

EXAMPLE OF RECONSTRUCTION



GROWTH DATA EXAMPLE



Yao et al.'s (2005) method with error term (top left), James and Hastie's (2001) method (bottom left), our old method (bottom right).

METHOD DESIGNED FOR FRAGMENTS (PART 2)

• In Delaigle and Hall (2016) model data by Markov chains.

- Discretise the process in time: t_1, \ldots, t_{m_1} and space: y_1, \ldots, y_{m_2} .
- Reduce data $X_i(t)$, $t \in \mathcal{I}_i$, to set of point pairs $(t_j, Z_i(t_j))$.
- Assume $P\{Z(t_{k+1}) = y_{\ell} \mid Z(t_k), \dots, Z(t_1)\} = P\{Z(t_{k+1}) = y_{\ell} \mid Z(t_k)\}.$
- For all k, j and ℓ , estimate $P\{Z(t_{k+1}) = y_{\ell} | Z(t_k) = y_j\}$.

IMPUTING MISSING PARTS OF CURVES

Z observed on $[A, B] \subset [a, b]$. Markov assumption implies

$$E\{Z(t)|Z(s), s \in [A,B]\} = \begin{cases} Z(t) & \text{if } t \in [A,B] \\ E\{Z(t)|Z(A)\} & \text{if } a \le t < A \\ E\{Z(t)|Z(B)\} & \text{if } B < t \le b . \end{cases}$$

• We have

$$E\left\{Z(t_{j+r}) \mid Z(t_{j}) = y_{j_{1}}\right\}$$

= $\sum_{\ell=1}^{m_{1}} \left\{\sum_{\text{paths from } y_{j_{1}} \text{ to } y_{j_{r}} = y_{\ell}} \prod_{k=1}^{r} P\left\{Z(t_{j+k}) = y_{j_{k+1}} | Z(t_{j+k-1}) = y_{j_{k}}\right\}\right\} y_{\ell}$

- Estimate using estimated transition probabilities.
- Use matrix formulation.

$GROWTH \ DATA \ EXAMPLE$



Yao et al.'s (2005) method with error term (top left), James and Hastie's (2001) method (bottom left), our new method (bottom right).

COVARIANCE ESTIMATION

• For covariance, use same ideas to estimate $E\left\{Z(t) Z(u) \middle| Z(s), s \in [A, B]\right\}$ $= \begin{cases}Z(t) Z(u) & \text{if } t, u \in [A, B]\\Z(t) E\{Z(u) \mid Z(s), s \in [A, B]\} & \text{if } t \in [A, B] \text{ but } u \notin [A, B]\\\text{etc}\end{cases}$

• If enough data to fit, can use higher order Markov assumption:

$$P\{Z(t_{k+r}) = y_{\ell} \mid Z(t_{k+r-1}), \dots, Z(t_1)\} = P\{Z(t_{k+r}) = y_{\ell} \mid Z(t_{k+r-1}), \dots, Z(t_k)\}.$$

OUR MORE RECENT IDEA

• Estimating *K* on $\mathcal{I} \times \mathcal{I}$ from fragments is only possible if we can identify *K* on $\mathcal{I} \times \mathcal{I}$ by knowing *K* on the diagonal band where we observe data.



Method

• In that case, we express *K* in an orthogonal series expansion:

$$K(s,t) = \sum_{j_1=1}^{\infty} \sum_{j_2=1}^{\infty} a_{j_1 j_2} \psi_{j_1}(s) \psi_{j_2}(t) .$$
(1)

- Then estimate the coefficients using only the diagonal band by minimising the distance between K and \hat{K} computed on the diagonal band.
- Minimise under the constraint that *K* is symmetric and semipositive definite on $\mathcal{I} \times \mathcal{I}$.
- Then use the resulting coefficients on the whole $\mathcal{I} \times \mathcal{I}$.

THEORY

- We have theoretical results giving conditions under which *K* is identifiable on $\mathcal{I} \times \mathcal{I}$ knowing only *K* on the diagonal band.
- One example is when the *X*_{*i*}'s are real analytic, see Descary and Panaretos (2017) for similar results using another method.
- We have more general results based on fast enough decay of eigenvalues. The larger the observed band, the better.
- We can also show that even if we do not have identifiability, we can have relatively small error of approximation.

Figure 1: n = 50, mean fragment length: 0.5. True (left) and estimated (right).



Figure 2: n = 50 (top) or 500 (bottom), mean fragment length: 0.2. True (left) and estimated (right).



References

- Bachrach, L. K., Hastie, T. J., Wang, M. C., Narasimhan, B. and Marcus, R. (1999). Bone mineral acquisition in healthy Asian, Hispanic, Black and Caucasian youth; a longitudinal study. *J. Clinical Endocrinology & Metabolism*, **84**, 4702–4712.
- Descary, M-H. and Panaretos, V. (2017). Recovering Covariance from Functional Fragments. *Manuscript*.
- Delaigle, A. and Hall, P. (2013). Classification using censored functional data. *J. Amer. Statist. Assoc.*, **108**, 1269–1283.
- Delaigle, A. and Hall, P. (2016). Approximating fragmented functional data by segments of Markov chains. *Biometrika*, **103**, 779–799.
- James, G. and Hastie, T. (2001). Functional linear discriminant analysis for irregularly sampled curves. *J. Roy. Statist. Soc.*, Ser. B, **63**, 533–550.
- Yao, F., Müller, H. G. and Wang, J. L. (2005). Functional data analysis for sparse longitudinal data. *J. Amer. Statist. Assoc.*, **100**, 577–590