Local Bayesian clustering for functional data

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Introduction

For standard Euclidean data, clustering is quite straightforward since a point may belong to only a cluster. On the other hand, for functional data the problem becomes more complex since one may perform

- **clustering at global level**: a whole function is assigned to a single cluster,
- **clustering at local level**: the same function may belong to different clusters depending on the point of its domain at which it is evaluated.

Goal: performing local clustering for functional data.

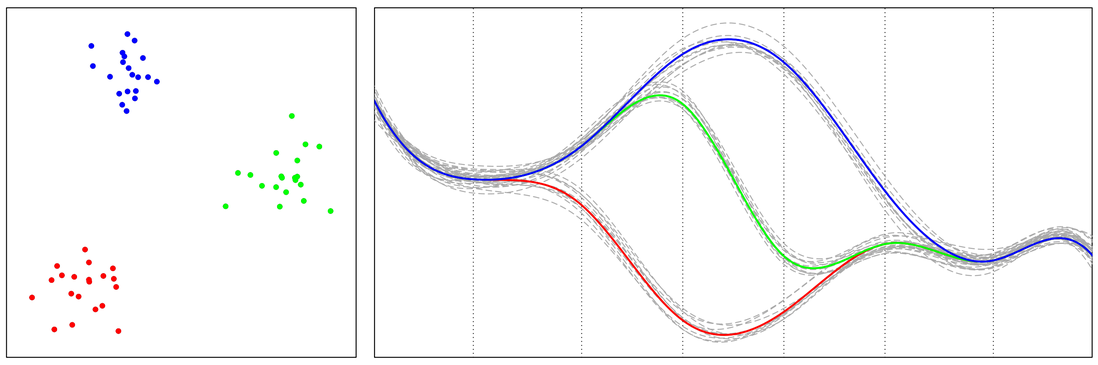


Figure 1: Comparison of a clustering problem for non-functional and functional data.

Contributions

We propose a Bayesian approach for the analysis of functional data that

- exploits the local property of B-spline basis expansion to perform indirect local clustering,
- defines **unit-specific B-spline parameters in terms of unit- and basis-specific cluster assignments**,
- employs an **ad-hoc definition for contiguous cluster-specific parameters ensuring smooth functions**,
- employs a novel **dependent random partition model inducing sequences of random partitions exhibiting semi-Markovian dependence**.

Modeling expected values via B-spline basis expansion

We assume that a random curve $Y_i(x)$, evaluated at the point $x \in \mathbb{R}$, follows

$$Y_i(x) \mid \boldsymbol{\theta}^*, \mathbf{c}_i, \sigma^2 \overset{ind}{\sim} \mathsf{N}\left(\boldsymbol{b}(x)^\top \boldsymbol{\theta}_i, \sigma^2\right),$$

where $\boldsymbol{b}(x)$ is a d-degree B-spline with basis coefficient

$$\boldsymbol{\theta}_i = (\theta^*_{1,c_{i,1}}, \ldots, \theta^*_{K,c_{i,K}}),$$

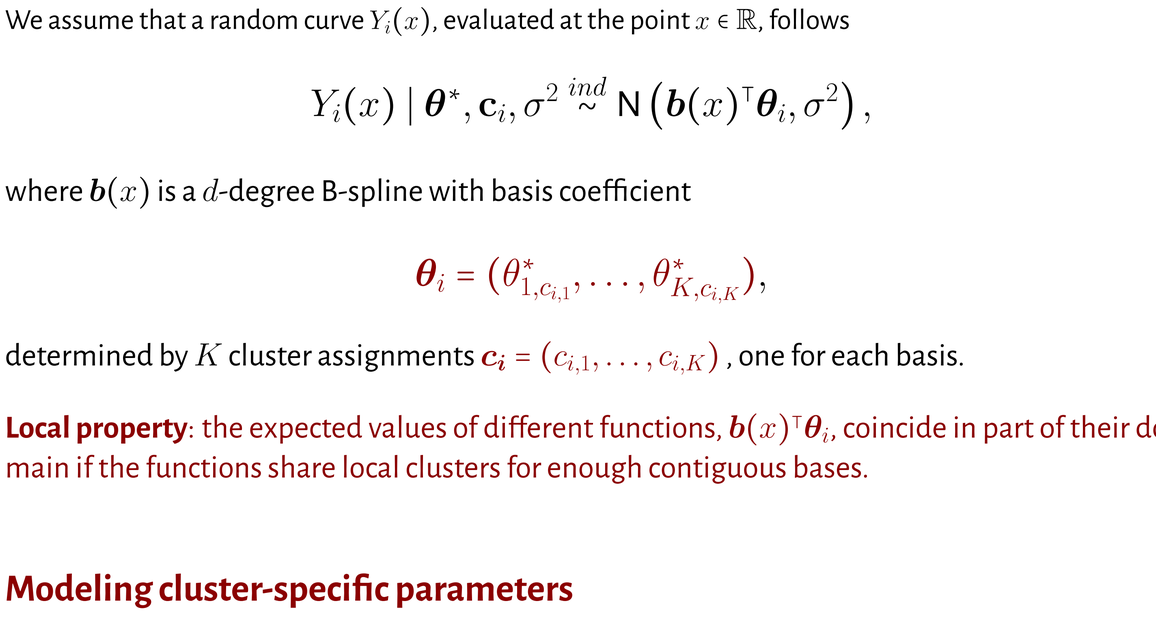
determined by K cluster assignments $\boldsymbol{c_i} = (c_{i,1}, \ldots, c_{i,K})$, one for each basis.

Local property: the expected values of different functions, $\boldsymbol{b}(x)^\top \boldsymbol{\theta}_i$, coincide in part of their domain if the functions share local clusters for enough contiguous bases.

Modeling cluster-specific parameters

We consider a partition of the curves at each basis, ρ_k, and define the cluster-specific parameters is such a way that contiguous parameters in each $\boldsymbol{\theta}_i$ are similar:

$$\theta^*_{kj} \mid \boldsymbol{\theta}^*_{k-1}, \rho_k, \rho_{k-1}, \phi, \tau^2 \overset{ind}{\sim} \mathsf{N}\left(\frac{\phi}{|C^{(\to j)}_{k-1}|} \sum_{l \in C^{(\to j)}_{k-1}} \theta^*_{k-1,l}, \tau^2\right).$$



Semi-Markovian Random Partition Model (smRPM)

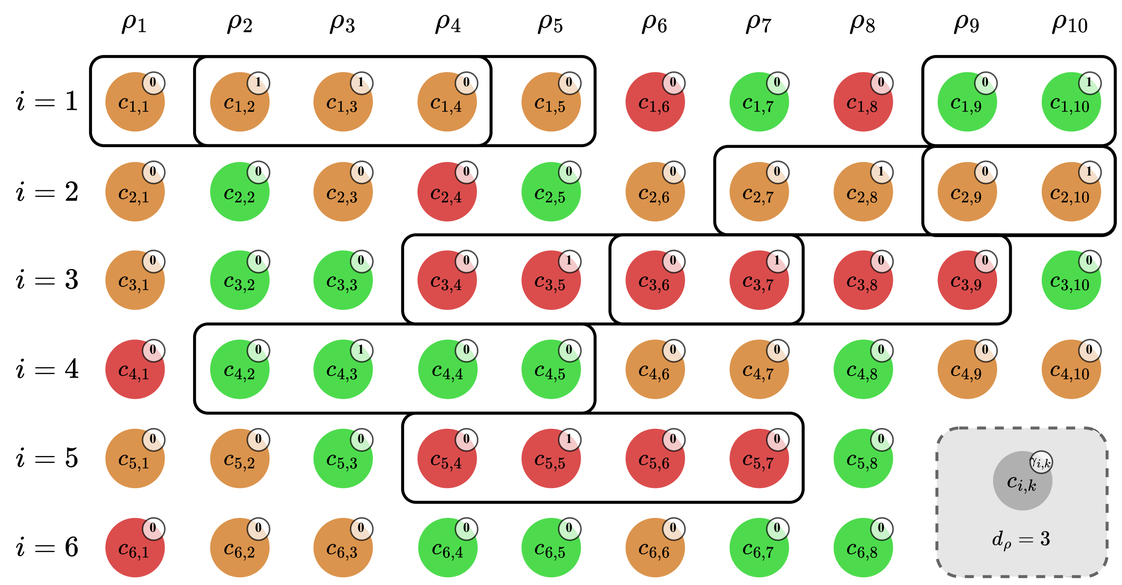
We introduce auxiliary variables explicitly modeling the evolution of the partitions at different basis:

$$\gamma_{ik} = \begin{cases} 1 & \text{if curve } i \textit{ cannot} \text{ be reallocated when moving from basis } k-1 \text{ to } k+d_\rho-1 \\ 0 & \text{otherwise} \end{cases}.$$

The distribution of the partition at basis k is influenced by the auxiliary variables related to bases $k, \ldots, k-d_\rho+1$, collected in $\boldsymbol{\gamma}^{(d_\rho)}_k$:

$$\Pr(\rho_k = \lambda \mid \boldsymbol{\gamma}^{(d_\rho)}_k, \rho_{k-1}) = \frac{\Pr(\rho_k = \lambda)\mathbb{I}\left(\lambda \in P_{\mathcal{R}_k}\right)}{\sum_{\lambda' \in P} \Pr(\rho_k = \lambda')\mathbb{I}\left(\lambda' \in P_{\mathcal{R}_k}\right)},$$

where $P_{\mathcal{R}_k}$ is the set of partitions that are compatible with ρ_{k-1} based on $\boldsymbol{\gamma}^{(d_\rho)}_k$.



The probabilities of success of the auxiliary variables at different basis can be independent,

$$\gamma_{ik} \mid \alpha_k \overset{ind}{\sim} \mathsf{Ber}(\alpha_k),$$
$$\alpha_k \overset{iid}{\sim} \mathsf{Beta}(a_\alpha, b_\alpha),$$

or have d_γ-order dependence,

$$\gamma_{ik} \mid \boldsymbol{\alpha}, \boldsymbol{\gamma}^{(d_\gamma)}_{i,k-1} \overset{ind}{\sim} \mathsf{Ber}\left(\pi\left(\alpha_0 + \alpha_1 \sum_{q=1}^{d_\gamma} \gamma_{i,k-q}\right)\right),$$
$$\boldsymbol{\alpha} \sim \mathsf{N}_2(\mathbf{a}, \mathbf{A}), \quad \omega_{ik} \overset{iid}{\sim} \mathsf{PG}(0,1). \qquad \text{(Polson et al. (2013))}$$

Notation: assuming $\rho_1 \sim \mathrm{CRP}(M)$, the model is denoted as $\mathrm{smRPM}_{d_\rho,d_\gamma}(\boldsymbol{\alpha}, M)$.

If $d_\rho = 1, d_\gamma = 0$, the model coincides with temporal Random Partition Model (Page et al., 2022).

Simulations

We define $n^{(ref)} = 5$ reference functional observations with known cluster assignments, and we simulate $R = 50$ datasets containing $n^{(rep)} \in \{10, 30\}$ realizations of each of these reference functional observations.

We simulate the observations and the cluster-specific parameters as

$$Y_i(x) \mid \boldsymbol{\theta}^*, \mathbf{c}_i, \sigma^2 \overset{ind}{\sim} \mathsf{N}\left(\boldsymbol{b}(x)^\top \boldsymbol{\theta}_i, \sigma^2\right),$$
$$\theta^*_{1j} \overset{ind}{\sim} (10j, 5), \quad \theta^*_{kj} \mid \boldsymbol{\theta}^*_{k-1}, \rho_k, \rho_{k-1} \overset{ind}{\sim} \left(\frac{1}{|C^{(\to j)}_{k-1}|} \sum_{l \in C^{(\to j)}_{k-1}} \theta^*_{k-1,l}, 5\right),$$

where $\sigma^2 \in \{1, 4\}$ quantifies the noise added to the reference functional observations.

Evaluation: Adjusted Rand Index (Hubert and Arabie, 1985) computed on each MCMC iteration.

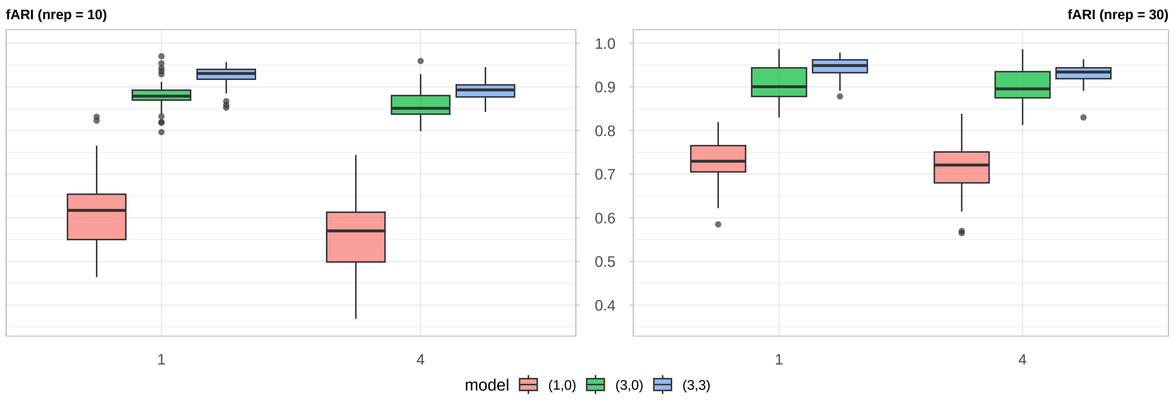


Figure 2: Boxplot of the average posterior ARI across the sequence of partitions computed on $R = 50$ simulated datasets.

References

Page, G. L., Quintana, F. A., Dahl, D. B. (2022). Dependent Modeling of Temporal Sequences of Random Partitions. In: Journal of Computational and Graphical Statistics, **31 (2)**, 614–627.

Hubert, L., and Arabie, P. (1985). Comparing Partitions. In: Journal of Classification, **2**, 193–218.

Polson, N. G., Scott, J. G., Windle, J. (2013). Bayesian inference for logistic models using pólya–gamma latent variables. In: Journal of the American Statistical Association, **108 (504)**, 1339–1349..