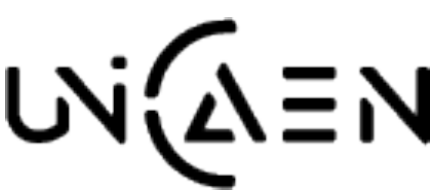
Unsupervised learning from high-dimensional and functional data

Faicel Chamroukhi




Research Summer School on Statistics for Data Science S4D 2018

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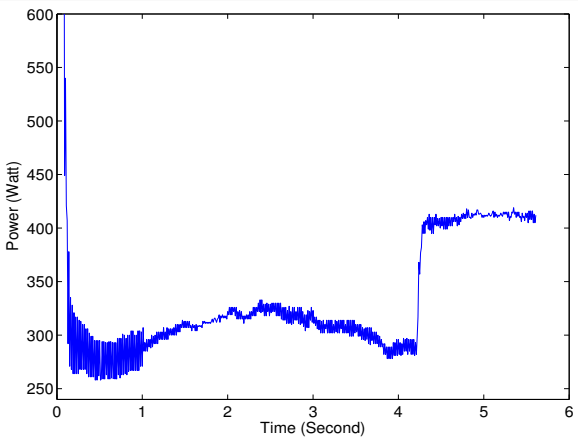
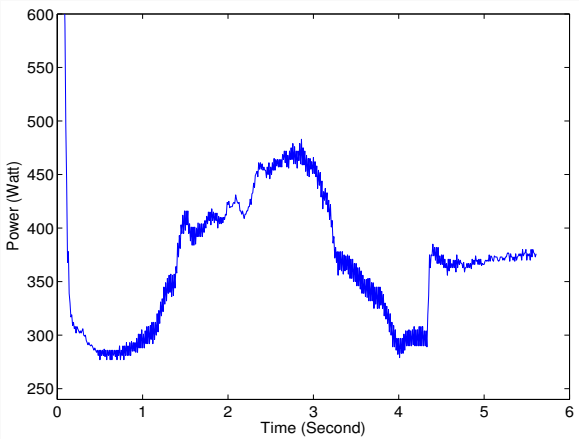
Temporal data

Temporal data with regime changes





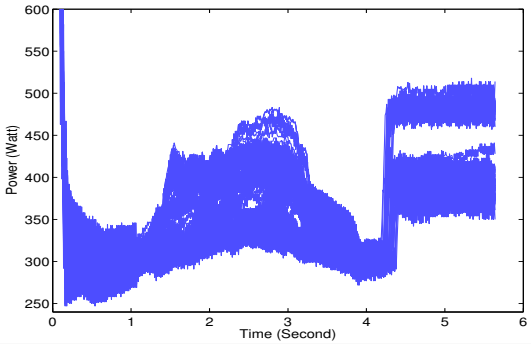
- Data with regime changes over time
- Abrupt and/or smooth regime changes

Objectives

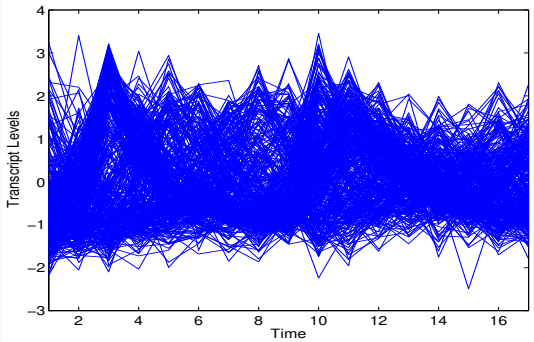
Temporal data modeling and segmentation

Functional data

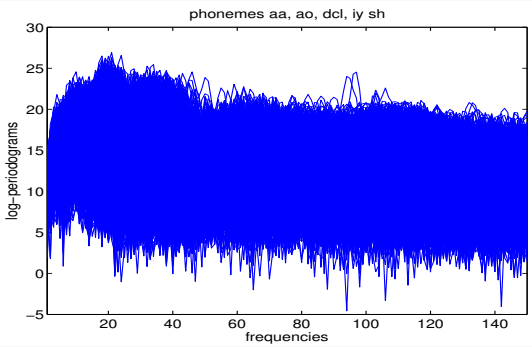
Many curves to analyze



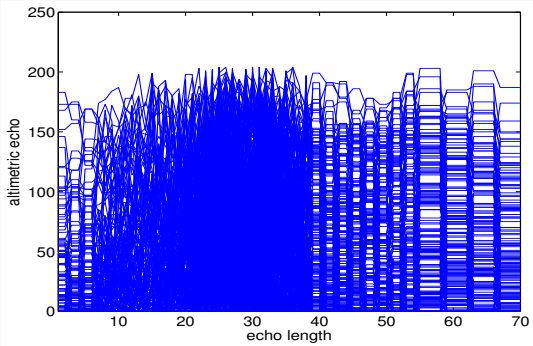
Railway switch curves



Yeast cell cycle curves



Phonemes curves



Satellite waveforms

Objectives

- Curve clustering/classification (functional data analysis framework)
- Deal with the problem of regime changes $\hookrightarrow$ Curve segmentation

Scientific context

- The area of statistical learning and analysis of complex data.
- **Data :** Complex data $\hookrightarrow$ *heterogeneous, temporal/dynamical, high-dimensional/functional, incomplete,...*
- **Objective:** Transform the data into knowledge :
  $\hookrightarrow$ Reconstruct hidden structure/information, groups/hierarchy of groups, summarizing prototypes, underlying dynamical processes, etc

Modeling framework

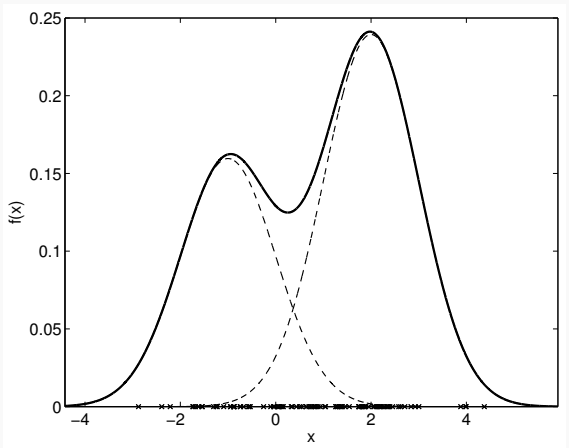
- Latent variable models : $f(x|\boldsymbol{\theta}) = \int_z f(x, z|\boldsymbol{\theta})\mathrm{d}z$
  Generative formulation :
$$\begin{aligned} z &\sim q(z|\boldsymbol{\theta}) \\ x|z &\sim f(x|z, \boldsymbol{\theta}) \end{aligned}$$

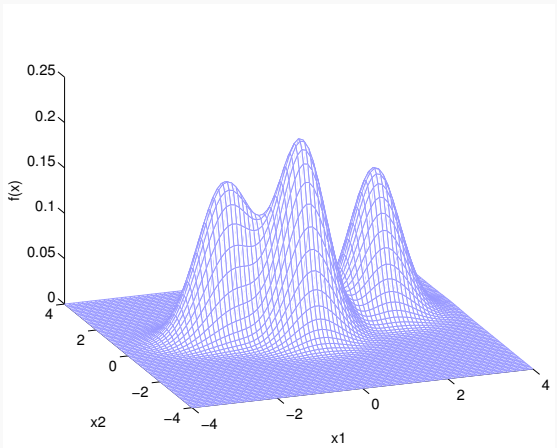
$\hookrightarrow$ Mixture models : $f(x|\boldsymbol{\theta}) = \sum_{k=1}^{K} \mathbb{P}(z = k) f(x|z = k, \boldsymbol{\theta}_k)$ and extensions

Mixture modeling framework

Mixture modeling framework

- Mixture density: $f(x|\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k f_k(x|\boldsymbol{\theta}_k)$





- Generative model

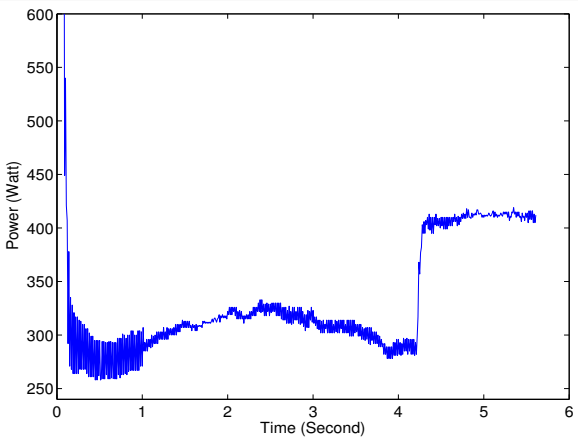
$$\begin{aligned} z &\sim \mathcal{M}(1; \pi_1, \ldots, \pi_K) \\ x|z &\sim f(x|\boldsymbol{\theta}_z) \end{aligned}$$

↪ Algorithms for inferring $\boldsymbol{\theta}$ from the data

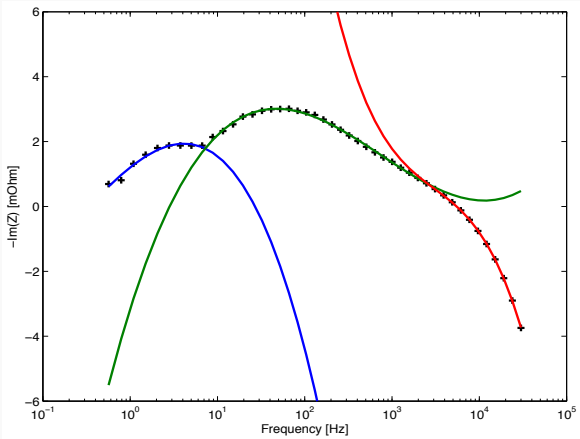
Outline

Outline

Temporal data with regime changes



Railway data



Energy data

Mixture models for temporal data segmentation

$\boldsymbol{y} = (y_1, \ldots, y_n)$ a time series of n univariate observations $y_i \in \mathbb{R}$ observed at the time points $\mathbf{t} = (t_1, \ldots, t_n)$

Times series segmentation context

- Time series segmentation is a popular problem with a broad literature
- Common problem for different communities, including statistics, detection, signal processing, machine learning, finance

- The observed time series is generated by an underlying process
  $\hookrightarrow$ segmentation $\equiv$ recovering the parameters the process' states.
- Conventional solutions are subject to limitations in the control of the transitions between these states

- $\hookrightarrow$ Propose generative latent data modeling for segmentation and approximation
- $\hookrightarrow$ segmentation $\equiv$ inferring the model parameters and the underlying

Regression with hidden logistic process

Let $\boldsymbol{y} = (y_1, \ldots, y_n)$ be a time series of n univariate observations $y_i \in \mathbb{R}$ observed at the time points $\mathbf{t} = (t_1, \ldots, t_n)$ governed by K regimes.

The Regression model with Hidden Logistic Process (RHLP) [1]

$$\begin{aligned} y_i &= \boldsymbol{\beta}_{z_i}^T \boldsymbol{x}_i + \sigma_{z_i} \epsilon_i \quad ; \quad \epsilon_i \sim \mathcal{N}(0,1), \quad (i = 1, \ldots, n) \\ Z_i &\sim \mathcal{M}(1, \pi_1(t_i; \mathbf{w}), \ldots, \pi_K(t_i; \mathbf{w})) \end{aligned}$$

Polynomial segments $\boldsymbol{\beta}_{z_i}^T \boldsymbol{x}_i$ with $\boldsymbol{x}_i = (1, t_i, \ldots, t_i^p)^T$ with logistic probabilities

$$\pi_k(t_i; \mathbf{w}) = \mathbb{P}(Z_i = k | t_i; \mathbf{w}) = \frac{\exp(w_{k1} t_i + w_{k0})}{\sum_{\ell=1}^{K} \exp(w_{\ell 1} t_i + w_{\ell 0})}$$

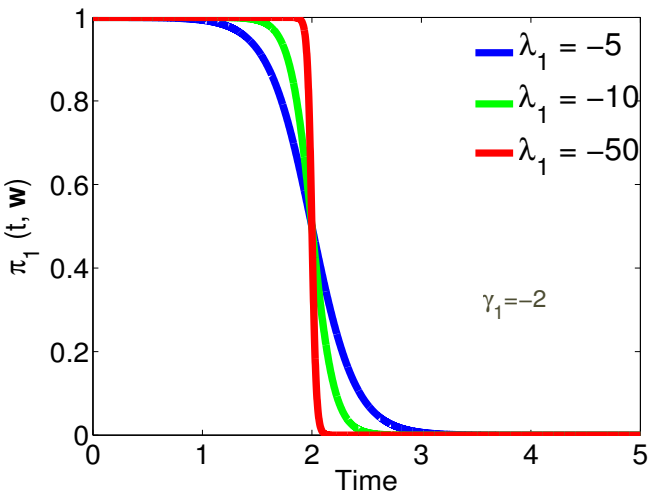
$$f(y_i | t_i; \boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k(t_i; \mathbf{w}) \mathcal{N}(y_i; \boldsymbol{\beta}_k^T \boldsymbol{x}_i, \sigma_k^2)$$

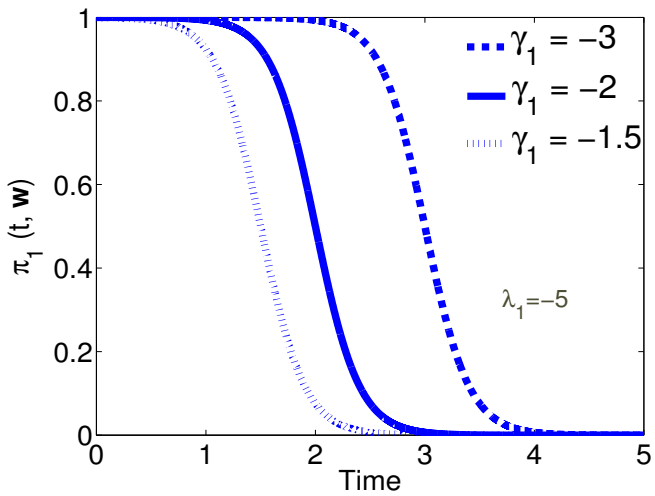
- Both the mixing proportions and the component parameters are time-varying
- Parameter vector of the model :$\boldsymbol{\theta} = (\mathbf{w}^T, \boldsymbol{\beta}_1^T, \ldots, \boldsymbol{\beta}_K^T, \sigma_1^2, \ldots, \sigma_K^2)^T$

Illustration

- Modeling with the logistic distribution allows activating simultaneously and preferentially several regimes during time

$$\pi_k(t_i; \mathbf{w}) = \frac{\exp\left(\lambda_k(t_i+\gamma_k)\right)}{\sum_{\ell=1}^{K} \exp\left(\lambda_\ell(t_i+\gamma_\ell)\right)}$$



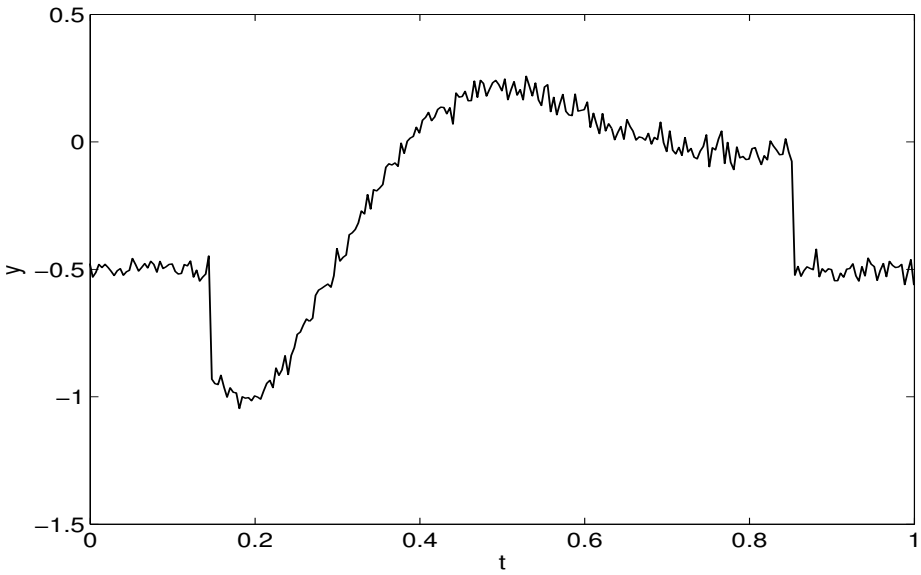


$\Rightarrow$ The parameter w_{k1} controls the quality of transitions between regimes

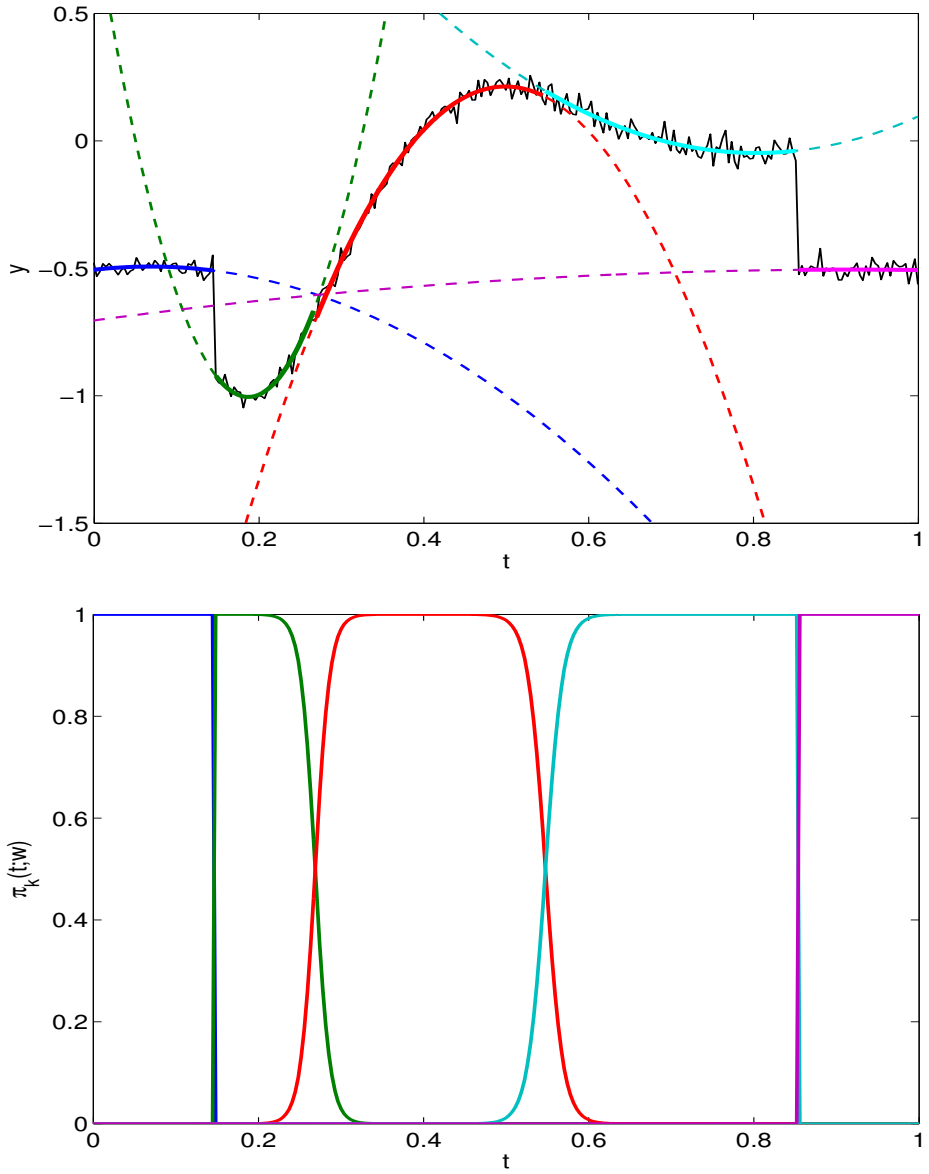
$\Rightarrow$ The parameter w_{k0} is related to the transition time point

- Ensure time series segmentation into contiguous segments

Illustration



Illustration



$K = 5$ polynomial components of degree $p = 2$

Parameter estimation: MLE via EM: EM-RHLP

- Parameter vector: $\boldsymbol{\theta} = (\mathbf{w}^T, \boldsymbol{\beta}_1^T, \ldots, \boldsymbol{\beta}_K^T, \sigma_1^2, \ldots, \sigma_K^2)^T$
- Maximize the observed-data log-likelihood:

$$\log L(\boldsymbol{\theta}; \boldsymbol{y}, \mathbf{t}) = \sum_{i=1}^{n} \log \sum_{k=1}^{K} \pi_k(t_i; \mathbf{w}) \mathcal{N}\left(y_i; \boldsymbol{\beta}_k^T \boldsymbol{x}_i, \sigma_k^2\right)$$

- Complete-data log-likelihood

$$\log L_c(\boldsymbol{\theta}; \boldsymbol{y}, \mathbf{t}, \mathbf{z}) = \sum_{i=1}^{n} \sum_{k=1}^{K} Z_{ik} \log[\pi_k(t_i; \mathbf{w}) \mathcal{N}\left(y_i; \boldsymbol{\beta}_k^T \boldsymbol{x}_i, \sigma_k^2\right)]$$

$Z_{ik} = 1$ if $Z_i = k$ (i.e., when y_i belongs to the kth component)

- The Q-function

$$\begin{aligned} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(q)}) &= \mathbb{E}\left[\log L_c(\boldsymbol{\theta}; \boldsymbol{y}, \mathbf{t}, \mathbf{z}) | \boldsymbol{y}, \mathbf{t}; \boldsymbol{\theta}^{(q)}\right] \\ &= \sum_{i=1}^{n} \sum_{k=1}^{K} \tau_{ik}^{(q)} \left[\log \pi_k(t_i; \mathbf{w}) \mathcal{N}\left(y_i; \boldsymbol{\beta}_k^T \boldsymbol{x}_i, \sigma_k^2\right)\right] \end{aligned}$$

EM-RHLP

- **E-Step**: compute the posterior component memberships:

$$\tau_{ik}^{(q)} = \mathbb{P}(Z_i = k | y_i, t_i; \boldsymbol{\theta}^{(q)}) = \frac{\pi_k(t_i; \mathbf{w}^{(q)}) \mathcal{N}(y_i; \boldsymbol{\beta}_k^{T(q)} \boldsymbol{x}_i, \sigma_k^{2(q)})}{\sum_{\ell=1}^{K} \pi_\ell(t_i; \mathbf{w}^{(q)}) \mathcal{N}(y_i; \boldsymbol{\beta}_\ell^{T(q)} \boldsymbol{x}_i, \sigma_\ell^{2(q)})} .$$

- **M-Step**: compute the parameter update $\boldsymbol{\theta}^{(q+1)} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(q)})$

$$\boldsymbol{\beta}_k^{(q+1)} = \Big[\sum_{i=1}^{n} \tau_{ik}^{(q)} \boldsymbol{x}_i \boldsymbol{x}_i^T \Big]^{-1} \sum_{i=1}^{n} \tau_{ik}^{(q)} y_i \boldsymbol{x}_i \quad \text{weighted polynomial regression}$$

$$\sigma_k^{2(q+1)} = \frac{1}{\sum_{i=1}^{n} \tau_{ik}^{(q)}} \sum_{i=1}^{n} \tau_{ik}^{(q)} (y_i - \boldsymbol{\beta}_k^{T(q+1)} \boldsymbol{x}_i)^2$$

$$\mathbf{w}^{(q+1)} = \arg\max_{\mathbf{w}} \sum_{i=1}^{n} \sum_{k=1}^{K} \tau_{ik}^{(q)} \log \pi_k(t_i; \mathbf{w}) \quad \text{weighted logistic regression}$$

EM-RHLP algorithm

M-Step: Weighted multi-class logistic regression

$$\mathbf{w}^{(q+1)} = \arg\max_{\mathbf{w}} \sum_{i=1}^{n} \sum_{k=1}^{K} \tau_{ik}^{(q)} \log \pi_k(t_i; \mathbf{w})$$

- A convex optimization problem
- Solved with a multi-class Iteratively Reweighted Least Squares (IRLS) algorithm (Newton-Raphson)

$$\mathbf{w}^{(l+1)} = \mathbf{w}^{(l)} - \left[\frac{\partial^2 Q_{\mathbf{w}}(\mathbf{w}, \boldsymbol{\theta}^{(q)})}{\partial \mathbf{w} \partial \mathbf{w}^T}\right]^{-1}_{\mathbf{w}=\mathbf{w}^{(l)}} \frac{\partial Q_{\mathbf{w}}(\mathbf{w}, \boldsymbol{\theta}^{(q)})}{\partial \mathbf{w}}\Big|_{\mathbf{w}=\mathbf{w}^{(l)}}$$

- Analytic calculation of the Hessian and the gradient
- EM-RHLP algorithm complexity: $\mathcal{O}(I_{\text{EM}} I_{\text{IRLS}} K^3 p^3 n)$ (more advantageous than dynamic programming).

Time series approximation and segmentation

1. Approximation: a prototype mean curve

$$\hat{y}_i = \mathbb{E}[y_i|t_i;\hat{\boldsymbol{\theta}}] = \sum_{k=1}^{K} \pi_k(t_i;\hat{\mathbf{w}})\hat{\boldsymbol{\beta}}_k^T \boldsymbol{x}_i$$

$\hookrightarrow$ A smooth and flexible approximation thanks to the the logistic weights

$\hookrightarrow$ The RHLP can be used as nonlinear regression model $y_i = f(t_i;\boldsymbol{\theta}) + \epsilon_i$ by covering functions of the form $f(t_i;\boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k(t_i;\mathbf{w})\boldsymbol{\beta}_k^T \boldsymbol{x}_i$ [3]

2. Curve segmentation:

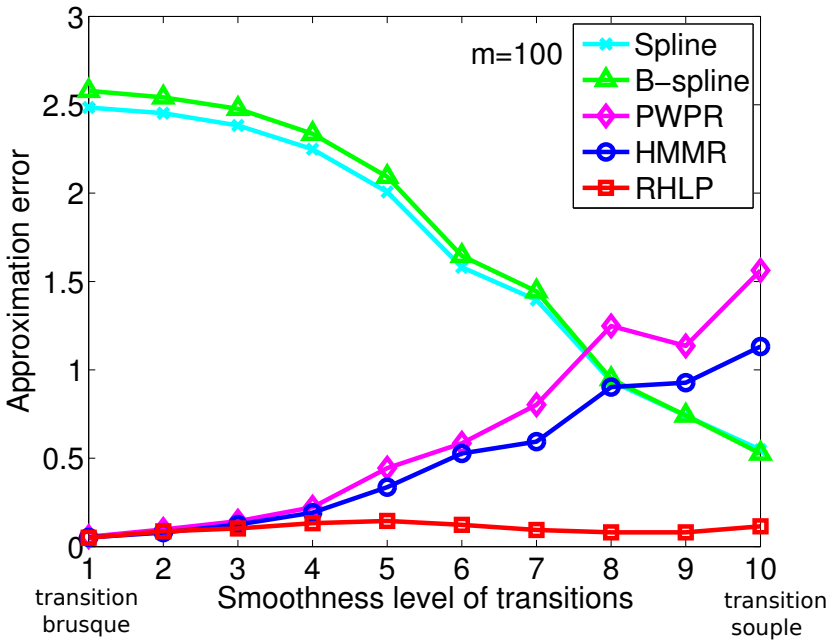
$$\hat{z}_i = \arg\max_{1\leq k\leq K} \mathbb{E}[z_i|t_i;\hat{\mathbf{w}}] = \arg\max_{1\leq k\leq K} \pi_k(t_i;\hat{\mathbf{w}})$$

3. **Model selection** Application of BIC, ICL

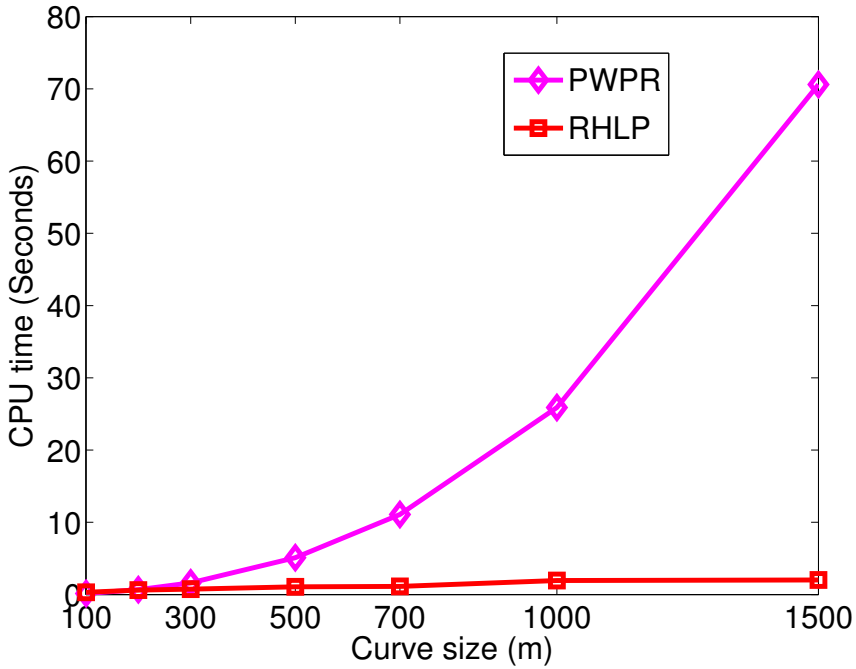
$\text{BIC}(K,p) = \log L(\hat{\boldsymbol{\theta}}) - \frac{\nu_{\boldsymbol{\theta}} \log(n)}{2}$; $\text{ICL}(K,p) = \log L_c(\hat{\boldsymbol{\theta}}) - \frac{\nu_{\boldsymbol{\theta}} \log(n)}{2}$ where $\nu_{\boldsymbol{\theta}} = K(p+4) - 2$.

Evaluation in modeling and segmentation

Approximation error as a function of the speed of transitions

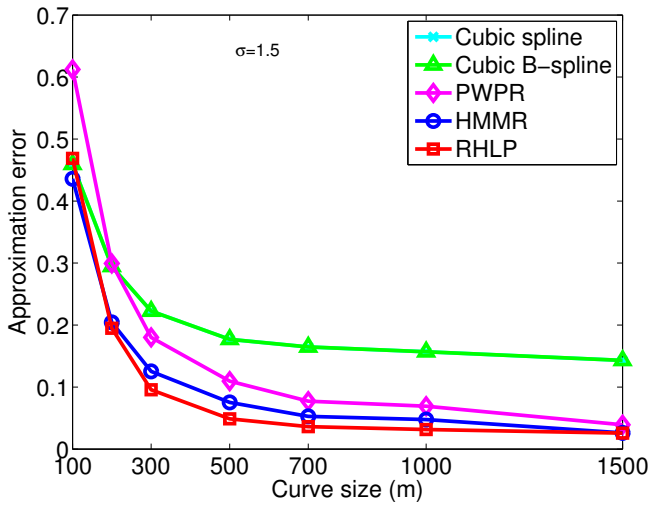


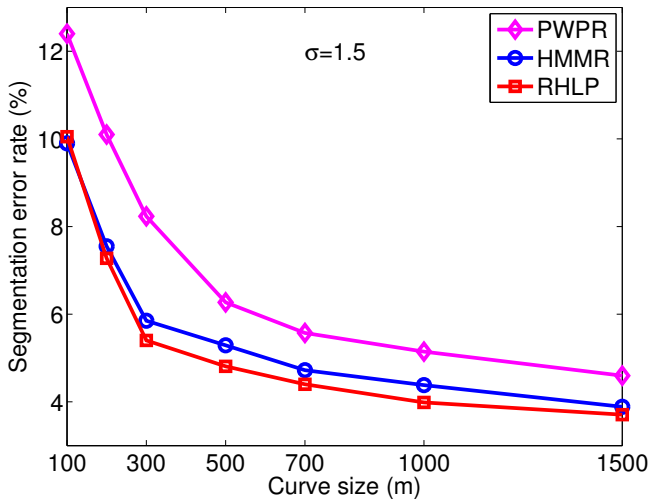
Computing time



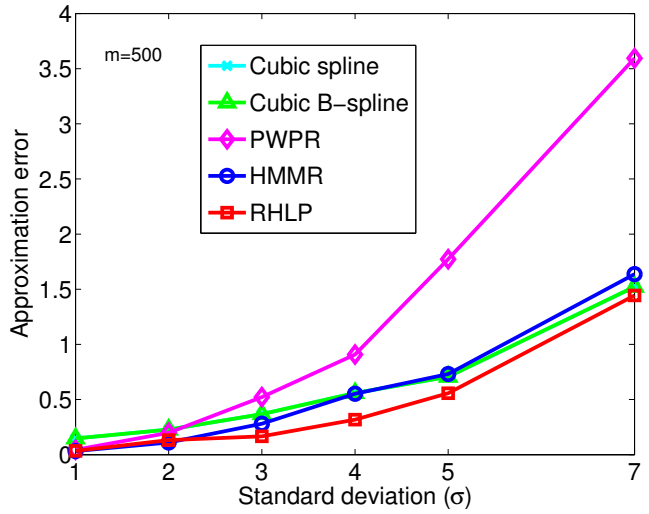
Evaluation in approximation and segmentation

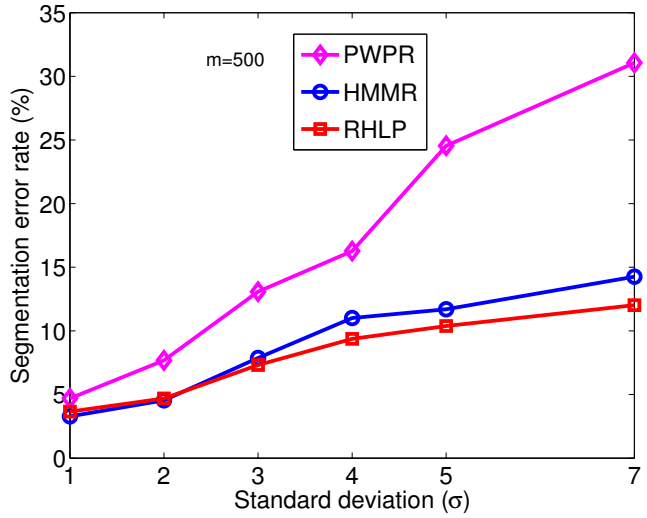
varying m



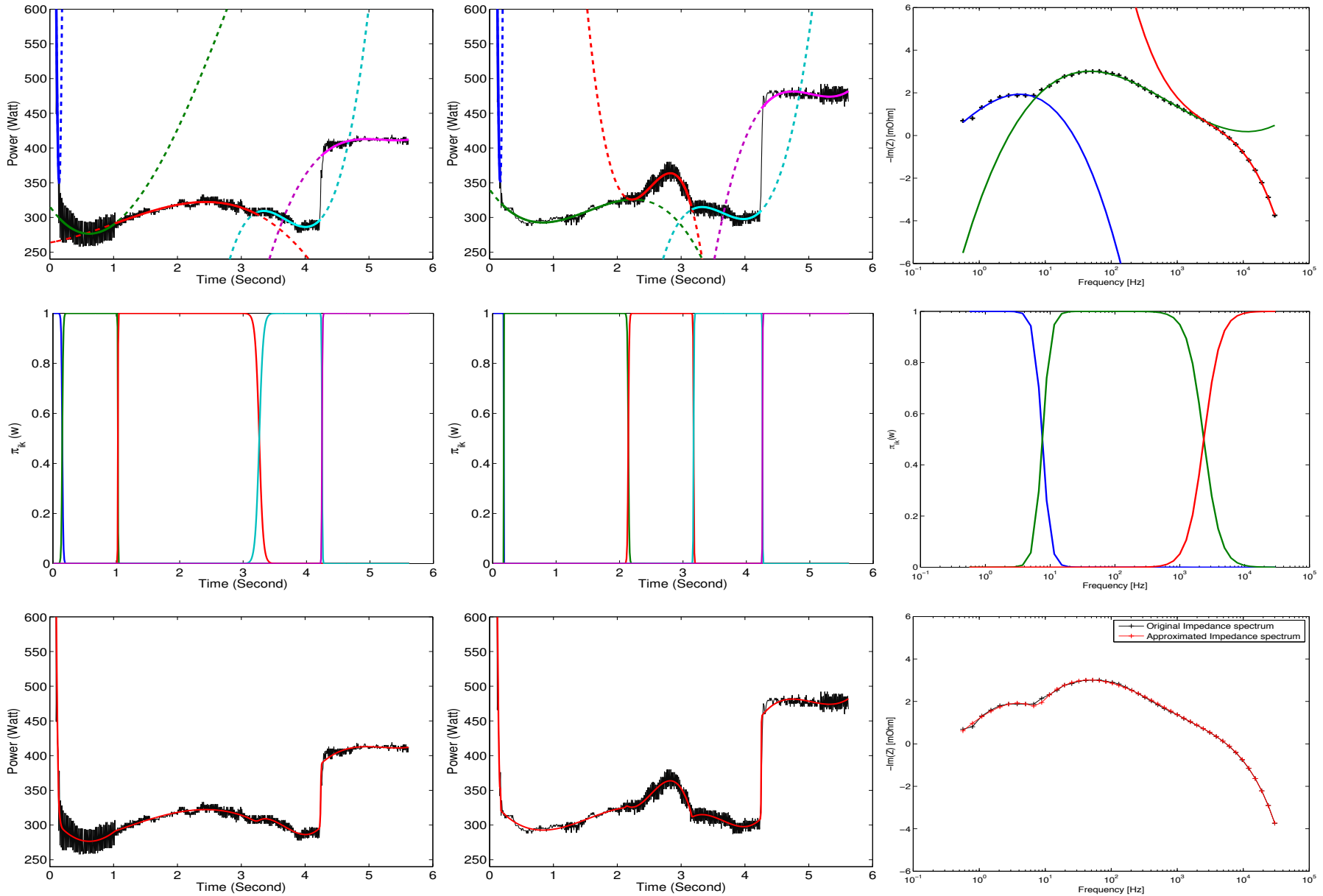


varying σ





Application to real data



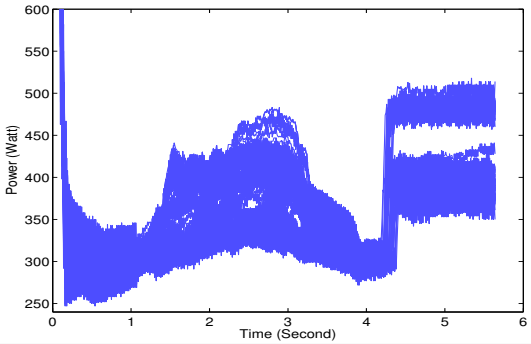
Outline

1. Mixture models for temporal data segmentation

2. Mixture models for functional data analysis
   - Mixture of piecewise regressions
   - Mixture of hidden logistic process regressions
   - Functional discriminant analysis

Functional data analysis context

Many curves to analyze



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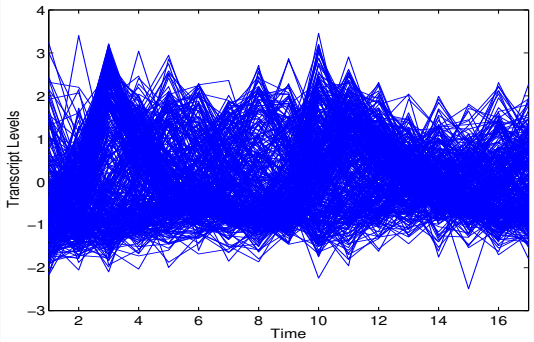

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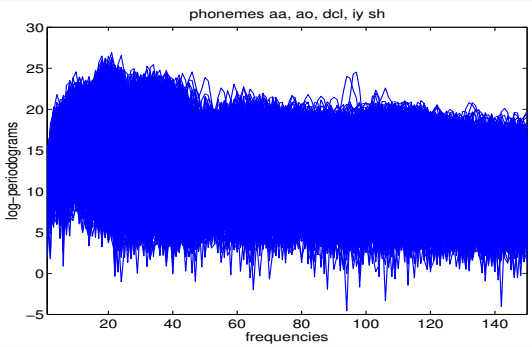

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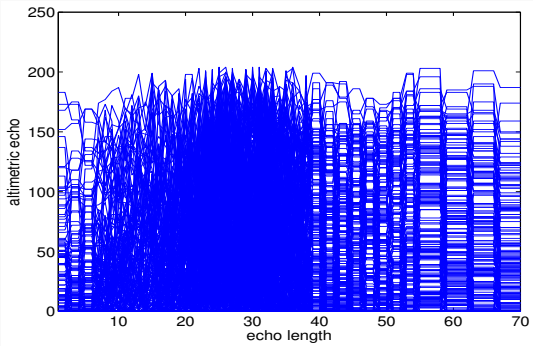


Satellite waveforms

Objectives

- Curve clustering/classification (functional data analysis framework)
- Deal with the problem of regime changes $\hookrightarrow$ Curve segmentation

Functional data analysis context

Data

- The individuals are entire functions (e.g., curves, surfaces)
- A set of n univariate curves $((\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{y}_n)$
- $(\boldsymbol{x}_i, \boldsymbol{y}_i)$ consists of m_i observations $\boldsymbol{y}_i = (y_{i1}, \ldots, y_{im_i})$ observed at the independent covariates, (e.g., time t in time series), $(x_{i1}, \ldots, x_{im_i})$

Objectives: exploratory or decisional

1. Unsupervised classification (clustering, segmentation) of functional data, particularly curves with regime changes: [4] [9], [C11] [16]
2. Discriminant analysis of functional data: [2], [5]

Functional data clustering/classification tools

- A broad literature (Kmeans-type, Model-based, etc)

  $\Rightarrow$ Mixture-model based cluster and discriminant analyzes

Mixture modeling framework for functional data

- The functional mixture model:

$$f(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\Psi}) \quad = \quad \sum_{k=1}^{K} \alpha_k f_k(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{\Psi}_k)$$

- $f_k(y|\boldsymbol{x})$ are tailored to functional data: can be polynomial (B-)spline regression, regression using wavelet bases etc, or Gaussian process regression, functional PCA

  $\hookrightarrow$ more tailored to approximate smooth functions

  $\hookrightarrow$ do not account for segmentation

Here $f_k(y|\boldsymbol{x})$ itself exhibits a clustering property via hidden variables (regimes):

1. Riecewise regression model (PWR)
2. Regression model with a hidden process (RHLP)

Piecewise regression mixture model (PWRM) [9]

- A probabilistic version of the K-means-like approach of (**?**)

$$f(\boldsymbol{y}_i|\boldsymbol{x}_i;\boldsymbol{\Psi}) = \sum_{k=1}^{K} \alpha_k \underbrace{\prod_{r=1}^{R_k} \prod_{j\in I_{kr}} \mathcal{N}(y_{ij};\boldsymbol{\beta}_{kr}^T\boldsymbol{x}_{ij},\sigma_{kr}^2)}_{\text{PWR}}$$

  $I_{kr} = (\xi_{kr}, \xi_{k,r+1}]$ are the element indexes of segment r for component k

- $\hookrightarrow$ Simultaneously accounts for curve clustering and segmentation
- Parameter vector $\boldsymbol{\Psi} = (\alpha_1, \ldots, \alpha_{K-1}, \boldsymbol{\theta}_1^T, \ldots, \boldsymbol{\theta}_K^T, \boldsymbol{\xi}_1^T, \ldots, \boldsymbol{\xi}_K^T)^T$ with $\boldsymbol{\theta}_k = (\boldsymbol{\beta}_{k1}^T, \ldots, \boldsymbol{\beta}_{kR_k}^T, \sigma_{k1}^2, \ldots, \sigma_{kR_k}^2)^T$ and $\boldsymbol{\xi}_k = (\xi_{k1}, \ldots, \xi_{k,R_k+1})^T$

Parameter estimation

1. Maximum likelihood estimation: EM-PWRM
2. Maximum classification likelihood estimation: CEM-PWRM

Maximum likelihood estimation via EM: EM-PWRM

- Maximize the observed-data log-likelihood:

$$\log L(\boldsymbol{\Psi}) = \sum_{i=1}^{n} \log \sum_{k=1}^{K} \alpha_k \prod_{r=1}^{R_k} \prod_{j \in I_{kr}} \mathcal{N}\left(y_{ij}; \boldsymbol{\beta}_{kr}^T \boldsymbol{x}_{ij}, \sigma_{kr}^2\right)$$

- The complete-data log-likelihood

$$\log L_c(\boldsymbol{\Psi}, \mathbf{z}) = \sum_{i=1}^{n} \sum_{k=1}^{K} Z_{ik} \log \alpha_k + \sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{R_k} \sum_{j \in I_{kr}} Z_{ik} \log \mathcal{N}(y_{ij}; \boldsymbol{\beta}_{kr}^T \boldsymbol{x}_{ij}, \sigma_{kr}^2)$$

- The conditional expected complete-data log-likelihood

$$Q(\boldsymbol{\Psi}, \boldsymbol{\Psi}^{(q)}) = \sum_{i=1}^{n} \sum_{k=1}^{K} \tau_{ik}^{(q)} \log \alpha_k + \sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{R_k} \sum_{j \in I_{kr}} \tau_{ik}^{(q)} \log \mathcal{N}(y_{ij}; \boldsymbol{\beta}_{kr}^T \boldsymbol{x}_{ij}, \sigma_{kr}^2)$$

EM-PWRM algorithm

E-step: Compute the $Q-$function

$\hookrightarrow$ Compute the posterior probability that the ith curve belongs to component k:

$$\tau_{ik}^{(q)} = \mathbb{P}(Z_i = k|\boldsymbol{y}_i, \boldsymbol{x}_i; \boldsymbol{\Psi}^{(q)}) = \frac{\alpha_k^{(q)} f_k\left(\boldsymbol{y}_i|\boldsymbol{x}_i;\boldsymbol{\Psi}_k^{(q)}\right)}{\sum_{k'=1}^{K} \alpha_{k'}^{(q)} f_{k'}\left(\boldsymbol{y}_i|\boldsymbol{x}_i;\boldsymbol{\Psi}_{k'}^{(q)}\right)}$$

M-step: Compute the update $\boldsymbol{\Psi}^{(q+1)} = \arg\max_{\boldsymbol{\Psi}} Q(\boldsymbol{\Psi}, \boldsymbol{\Psi}^{(q)})$

- $\alpha_k^{(q+1)} = \frac{\sum_{i=1}^{n} \tau_{ik}^{(q)}}{n}, \quad (k = 1, \ldots, K)$
- maximization w.r.t the piecewise regression parameters $\{\boldsymbol{\xi}_{kr}, \boldsymbol{\beta}_{kr}, \sigma_{kr}^2\}$ $\hookrightarrow$ a weighted piecewise regression problem $\hookrightarrow$ dynamic programming:

$$\begin{aligned}
\boldsymbol{\beta}_{kr}^{(q+1)} &= \left[\sum_{i=1}^{n} \tau_{ik}^{(q)} \mathbf{X}_{ir}^T \mathbf{X}_{ir}\right]^{-1} \sum_{i=1}^{n} \mathbf{X}_{ir} \boldsymbol{y}_{ir} \\
\sigma_{kr}^{2(q+1)} &= \frac{1}{\sum_{i=1}^{n} \sum_{j \in I_{kr}^{(q)}} \tau_{ik}^{(q)}} \sum_{i=1}^{n} \tau_{ik}^{(q)} \|\boldsymbol{y}_{ir} - \mathbf{X}_{ir} \boldsymbol{\beta}_{kr}^{(q+1)}\|^2
\end{aligned}$$

$\boldsymbol{y}_{ir}$ are the observations of segment r of the ith curve and $\mathbf{X}_{ir}$ its design matrix

Maximum classification likelihood estimation: CEM-PWRM

- Maximize the complete-data log-likelihood w.r.t $(\boldsymbol{\Psi}, \mathbf{z})$ simultaneously
- C-step: Bayes' optimal allocation rule: $\hat{z}_i = \arg\max_{1 \leq k \leq K} \tau_{ik}(\hat{\boldsymbol{\Psi}})$

CEM-PWRM is equivalent to the K-means-like algorithm of **?**:

$$\log L_c(\mathbf{z}, \boldsymbol{\Psi}) \propto \mathcal{J}\left(\mathbf{z}, \{\mu_{kr}, I_{kr}\}\right) = \sum_{k=1}^{K} \sum_{r=1}^{R_k} \sum_{i|Z_i=k} \sum_{j \in I_{kr}} \left(y_{ij} - \mu_{kr}\right)^2$$

if the following conditions hold:

- $\alpha_k = \frac{1}{K}\ \forall K$ (identical mixing proportions);
- $\sigma_{kr}^2 = \sigma^2\ \forall r$ and $\forall k$; (isotropic and homoskedastic model);
- μ_{kr}: piecewise *constant* regime approximation

- Curve clustering: $\hat{z}_i = \arg\max_k \tau_{ik}(\hat{\boldsymbol{\Psi}})$ with $\tau_{ik}(\hat{\boldsymbol{\Psi}}) = \mathbb{P}(Z_i | \boldsymbol{x}_i, \boldsymbol{y}_i; \hat{\boldsymbol{\Psi}})$
- Model selection: Application of BIC, ICL
- Complexity in $\mathcal{O}(I_{\text{EM}} K R n m^2 p^3)$: Significant computational load for large m

Simulation results

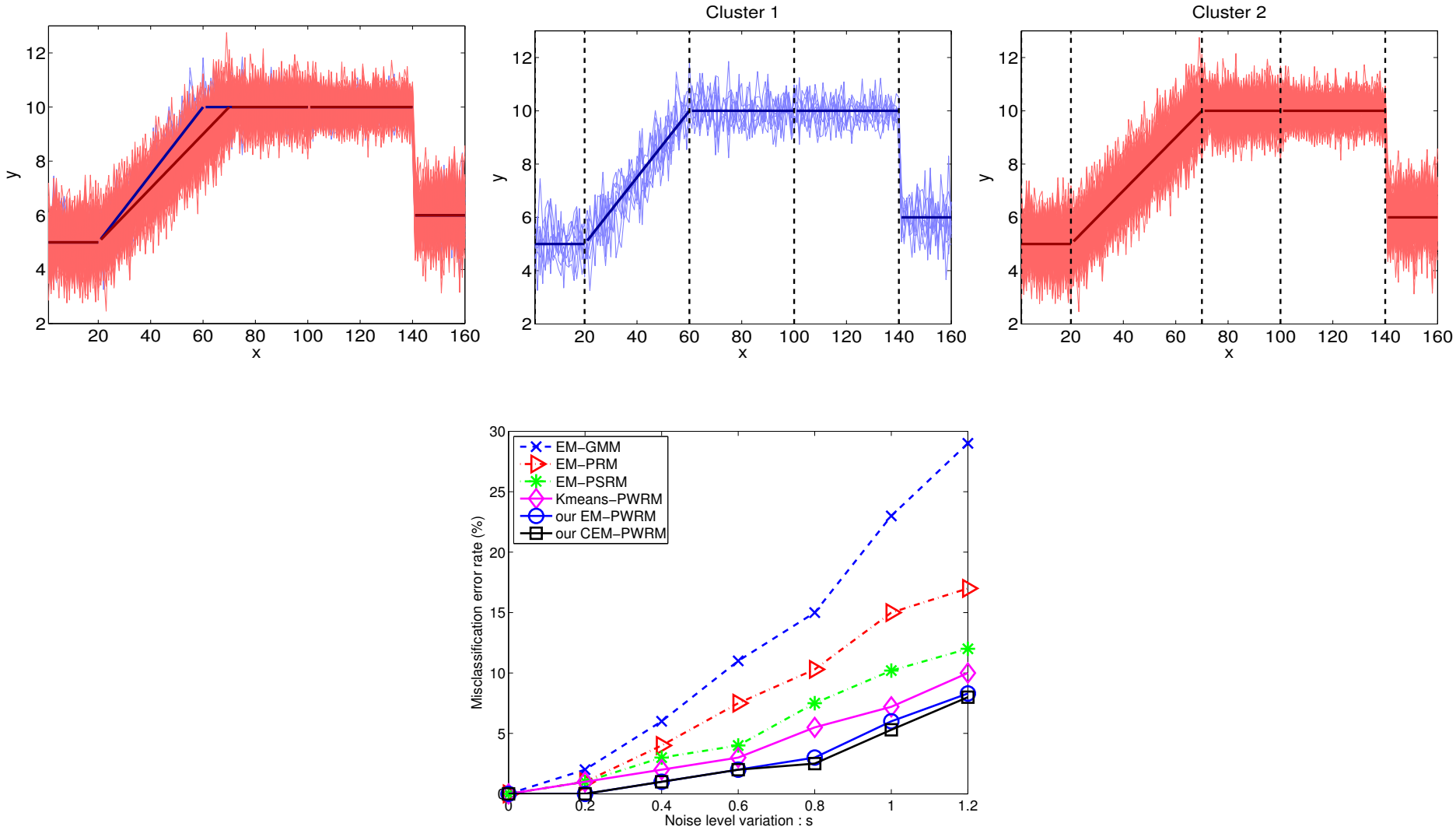
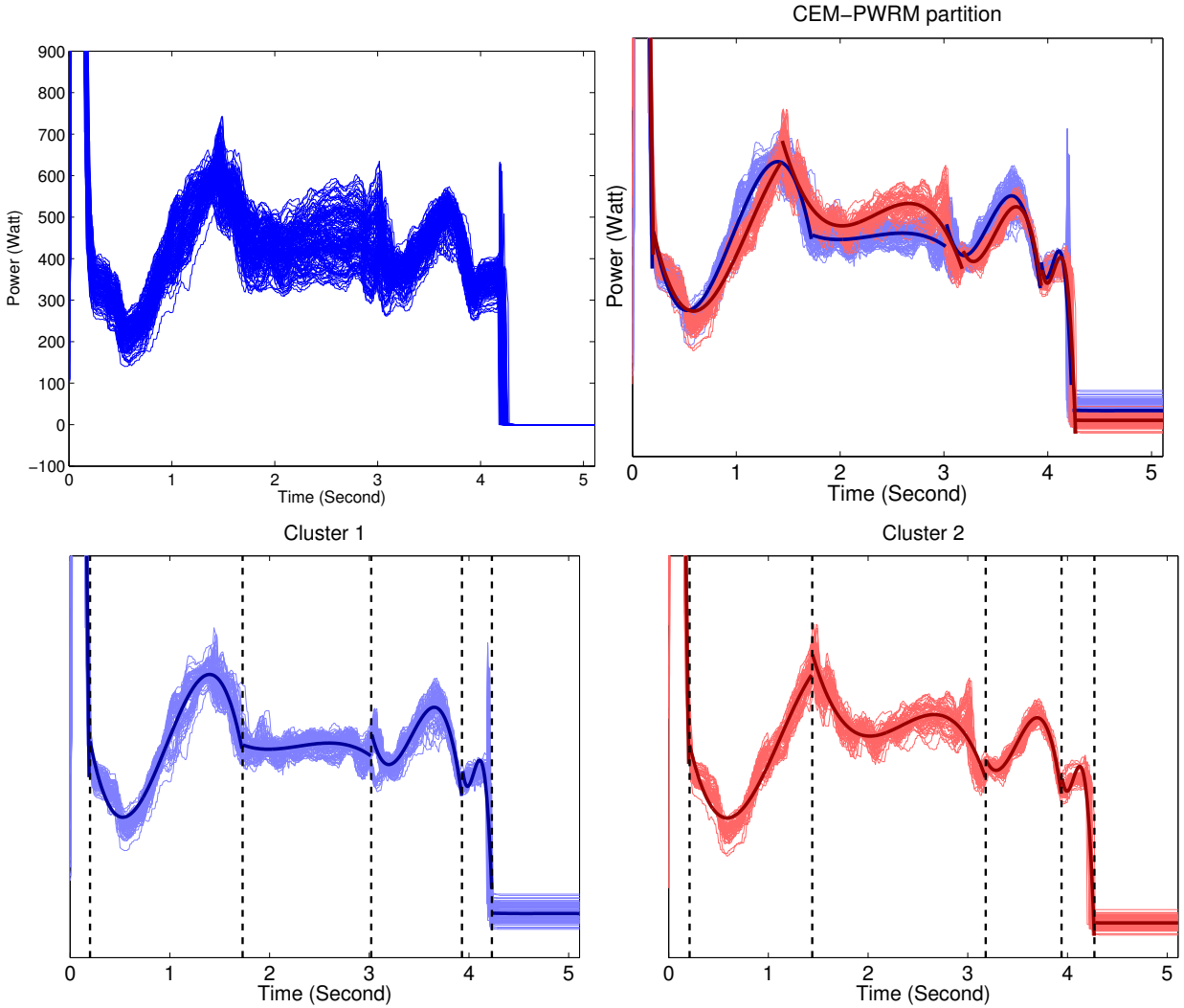


Figure: Misclassification error rate versus the noise level variation.

Application to switch operation curves

Data set: $n = 146$ real curves of $m = 511$ observations.

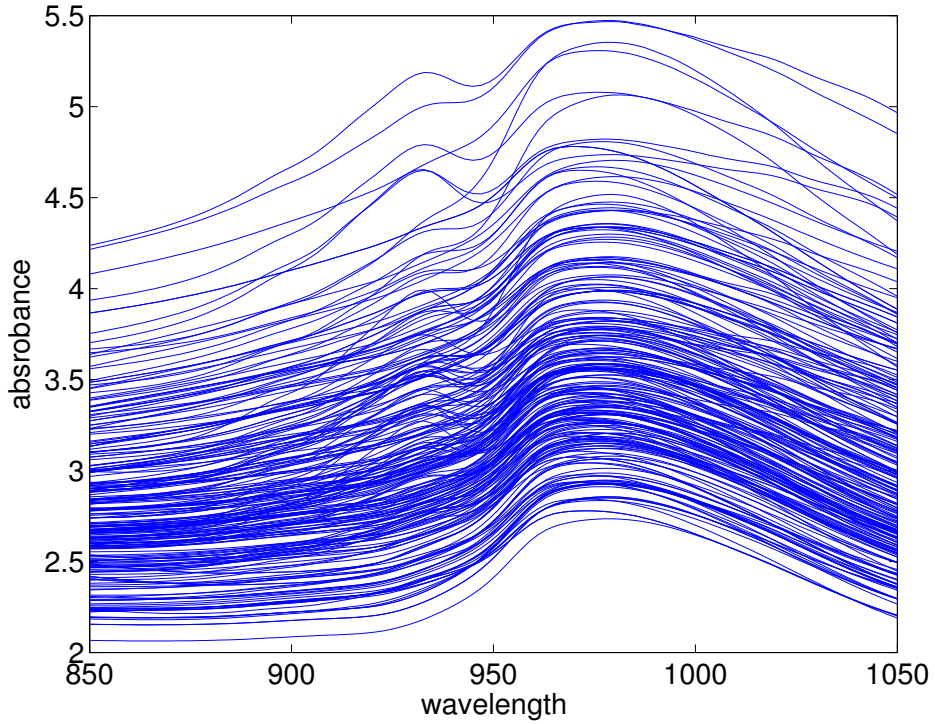
Each curve is composed of $R = 6$ electromechanical phases (regimes)



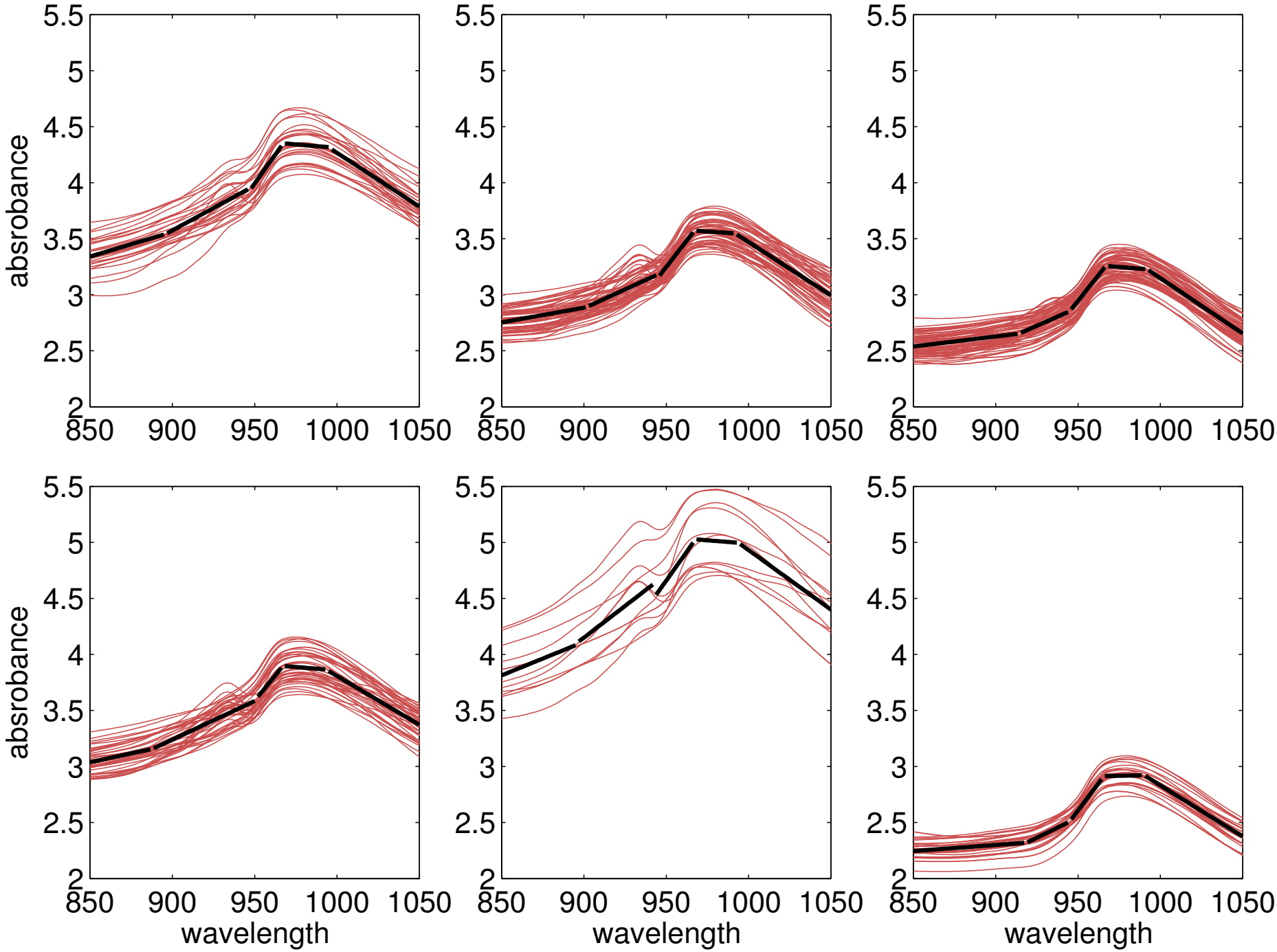
Application to Tecator data

The Tecator data set[1] contains $n = 240$ spectra with $m = 100$ observations for each spectrum

Data considered in the same setting as in **?** (six clusters, each cluster is approximated by five linear segments ($R = 5, p = 1$))

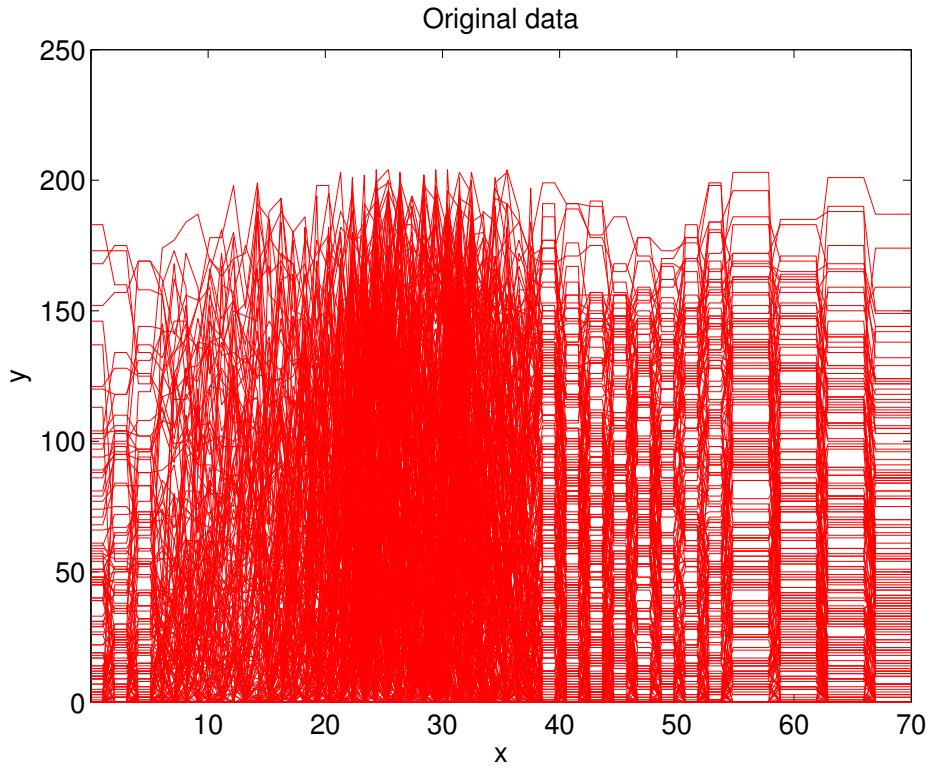


[1] Tecator data are available at `http://lib.stat.cmu.edu/datasets/tecator`.


absrobance
wavelength
5.5
5
4.5
4
3.5
3
2.5
2
850
900
950
1000
1050

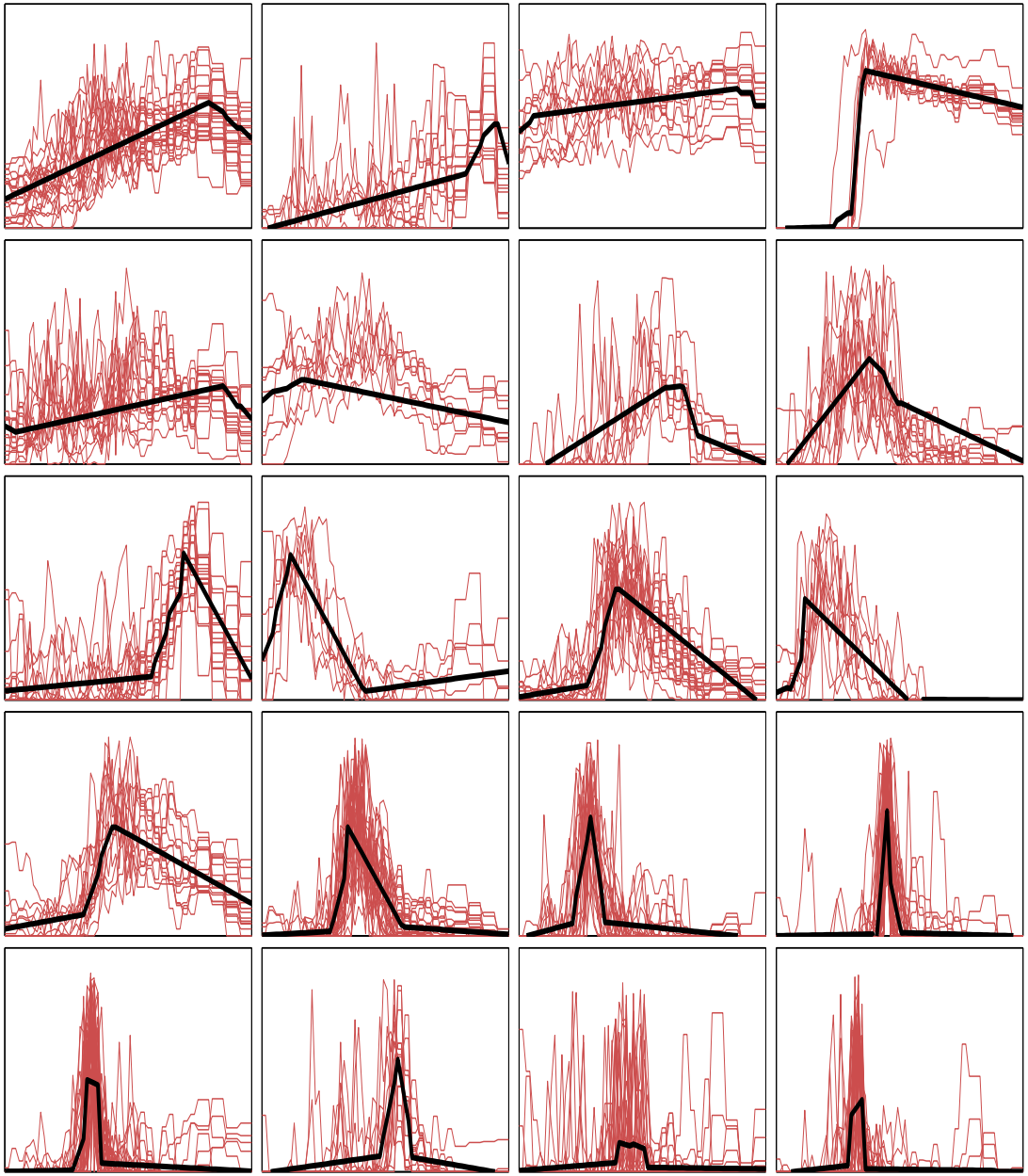
Topex/Poseidon satellite data

The Topex/Poseidon radar satellite data[2] contains $n = 472$ waveforms of the measured echoes, sampled at $m = 70$ (number of echoes)
We considered the same number of clusters (twenty) and a piecewise linear approximation of four segments per cluster as in **?**.



[2]Satellite data are available at
`http://www.lsp.ups-tlse.fr/staph/npfda/npfda-datasets.html`.

CEM-PWRM clustering



Summary

- Probabilistic approach to the simultaneous curve clustering and optimal segmentation
- Two algorithms: EM-PWRM and CEM-PWRM
- CEM-PWRM is a probabilistic-based version of the K-means-like algorithm **?**

- If the aim is density estimation, the EM version is suggested (CEM provides biased estimators but is well-tailored to the segmentation/clustering end)
- For continuous functions the PWRM in its current formulation, may lead to discontinuities between segments for the piecewise approximation.
- This may be avoided by posterior interpolation as in **?**.
- May lead to significant computational load especially for large time series. However, for quite reasonable dimensions, the algorithms remain usable

Mixture of hidden logistic process regressions [4]

- The mixture of regressions with hidden logistic processes (MixRHLP):

$$f(\boldsymbol{y}_i|\boldsymbol{x}_i;\boldsymbol{\Psi}) = \sum_{k=1}^{K} \alpha_k \underbrace{\prod_{j=1}^{m_i} \sum_{r=1}^{R_k} \pi_{kr}(x_j;\mathbf{w}_k)\mathcal{N}\left(y_{ij};\boldsymbol{\beta}_{kr}^T\boldsymbol{x}_j,\sigma_{kr}^2\right)}_{\text{RHLP}}$$

$$\pi_{kr}(x_j;\mathbf{w}_k) = \mathbb{P}(H_{ij}=r|Z_i=k,x_j;\mathbf{w}_k) = \frac{\exp\left(w_{kr0}+w_{kr1}x_j\right)}{\sum_{r'=1}^{R_k}\exp\left(w_{kr'0}+w_{kr'1}x_j\right)},$$

- Two types of component memberships:

  $\hookrightarrow$ cluster memberships (global) $Z_{ik}=1$ iff $Z_i=k$

  $\hookrightarrow$ regime memberships for a given cluster (local): $H_{ijr}=1$ iff $H_{ij}=r$

  MixRHLP deals better with the quality of regime changes

- Parameter estimation via the EM algorithm: EM-MixRHLP

MLE estimation via the EM algorithm

- The observed-data log-likelihood

$$\log L(\boldsymbol{\Psi}) = \sum_{i=1}^{n} \log \sum_{k=1}^{K} \alpha_k \prod_{j=1}^{m_i} \sum_{r=1}^{R_k} \pi_{kr}(x_j; \mathbf{w}_k) \mathcal{N}\left(y_{ij}; \boldsymbol{\beta}_{kr}^T \boldsymbol{x}_j, \sigma_{kr}^2\right)$$

- The complete-data log-likelihood:

$$\log L_c(\boldsymbol{\Psi}) = \sum_{i=1}^{n} \sum_{k=1}^{K} Z_{ik} \log \alpha_k + \sum_{i,j} \sum_{k=1}^{K} \sum_{r=1}^{R_k} Z_{ik} H_{ijr} \log \left[\pi_{kr}(x_j; \mathbf{w}_k) \mathcal{N}\left(y_{ij}; \boldsymbol{\beta}_{kr}^T \boldsymbol{x}_j, \sigma_{kr}^2\right)\right]$$

- The conditional expected complete-data log-likelihood

$$\begin{aligned} Q(\boldsymbol{\Psi}, \boldsymbol{\Psi}^{(q)}) &= \mathbb{E}\left[\log L_c(\boldsymbol{\Psi}) \middle| \mathcal{D}; \boldsymbol{\Psi}^{(q)}\right] \\ &= \sum_{i=1}^{n} \sum_{k=1}^{K} \tau_{ik}^{(q)} \log \alpha_k + \sum_{i,j} \sum_{k=1}^{K} \sum_{r=1}^{R_k} \tau_{ik}^{(q)} \gamma_{ijr}^{(q)} \log \left[\pi_{kr}(x_j; \mathbf{w}_k) \mathcal{N}\left(y_{ij}; \boldsymbol{\beta}_{kr}^T \boldsymbol{x}_j, \sigma_{kr}^2\right)\right]. \end{aligned}$$

EM-MixRHLP algorithm

E-step

- The posterior cluster memberships:

$$\tau_{ik}^{(q)} = \mathbb{P}(Z_i = k|\boldsymbol{y}_i, \boldsymbol{x}_i; \boldsymbol{\Psi}_k^{(q)}) = \frac{\alpha_k^{(q)} f(\boldsymbol{y}_i|Z_i = k, \boldsymbol{x}_i; \boldsymbol{\Psi}_k^{(q)})}{\sum_{k\prime=1}^{K} \alpha_{k'}^{(q)} f(\boldsymbol{y}_i|Z_i = k\prime, \boldsymbol{x}_i; \boldsymbol{\Psi}_{k\prime}^{(q)})}$$

- the posterior regime memberships:

$$\gamma_{ijr}^{(q)} = \mathbb{P}(H_{ij} = r|Z_i = k, y_{ij}, t_j; \boldsymbol{\Psi}_k^{(q)}) = \frac{\pi_{kr}(x_j; \mathbf{w}_k^{(q)}) \mathcal{N}(y_{ij}; \boldsymbol{\beta}_{kr}^{T(q)} \boldsymbol{x}_j, \sigma_{kr}^{2(q)})}{\sum_{r\prime=1}^{R_k} \pi_{kr\prime}(x_j; \mathbf{w}_k^{(q)}) \mathcal{N}(y_{ij}; \boldsymbol{\beta}_{kr\prime}^{T(q)} \boldsymbol{x}_j, \sigma_{kr\prime}^{2(q)})}$$

Computed directly (i.e, without a forward-backward recursion as in the Markovian model).

M-step of the EM-MixRHLP

M-step: calculate the update $\boldsymbol{\Psi}^{(q+1)} = \arg\max_{\boldsymbol{\Psi}} Q(\boldsymbol{\Psi}, \boldsymbol{\Psi}^{(q)})$.

- Mixing proportions update: standard

$$\alpha_k^{(q+1)} = \frac{1}{n}\sum_{i=1}^{n} \tau_{ik}^{(q)}, \quad (k = 1, \ldots, K).$$

- Regression parameters update: Analytic weighted least-squares problems

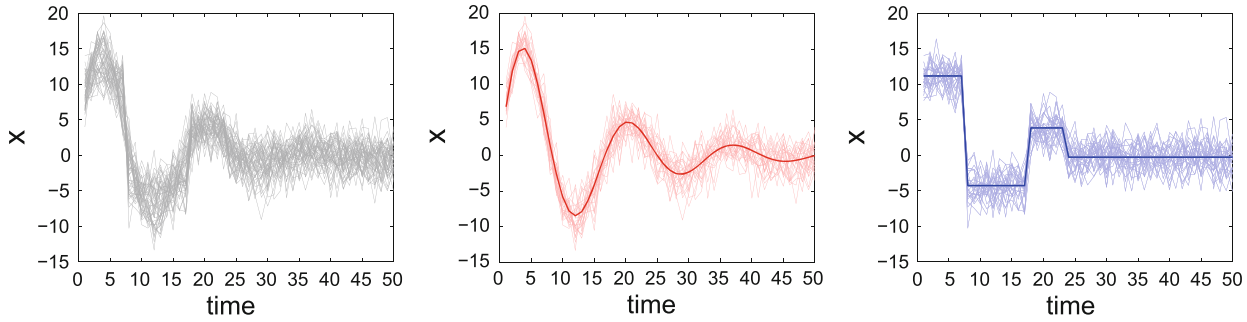
$$\boldsymbol{\beta}_{kr}^{(q+1)} = \Big[\sum_{i=1}^{n} \tau_{ik}^{(q)} \mathbf{X}_i^T \mathbf{W}_{ikr}^{(q)} \mathbf{X}_i\Big]^{-1} \sum_{i=1}^{n} \tau_{ik}^{(q)} \mathbf{X}_i^T \mathbf{W}_{ikr}^{(q)} \boldsymbol{y}_i,$$

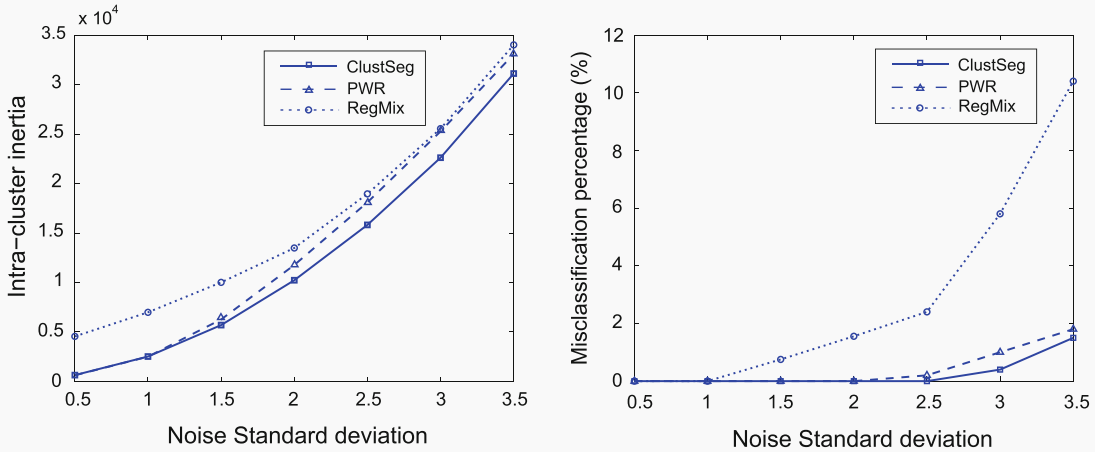
$$\sigma_{kr}^{2\ (q+1)} = \frac{\sum_{i=1}^{n} \tau_{ik}^{(q)} \| \sqrt{\mathbf{W}_{ikr}^{(q)}} (\boldsymbol{y}_i - \mathbf{X}_i \boldsymbol{\beta}_{kr}^{(q+1)}) \|^2}{\sum_{i=1}^{n} \tau_{ik}^{(q)} \text{trace}(\mathbf{W}_{ikr}^{(q)})},$$

  where $\mathbf{W}_{ikr}^{(q)} = \text{diag}(\gamma_{ijr}^{(q)}; j = 1, \ldots, m_i)$.

- Maximization w.r.t the logistic processes' parameters $\{\mathbf{w}_k\}$: solving multinomial logistic regression problems $\Rightarrow$ IRLS
- $\hookrightarrow$ EM-MixRHLP has complexity in $\mathcal{O}(I_{\text{EM}} I_{\text{IRLS}} K R^3 n m p^3)$ (K-means like algo. for PWR is in $\mathcal{O}(I_{\text{KM}} K R n m^2 p^3)$ $\hookrightarrow$ computationally attractive for large m with moderate value of R.

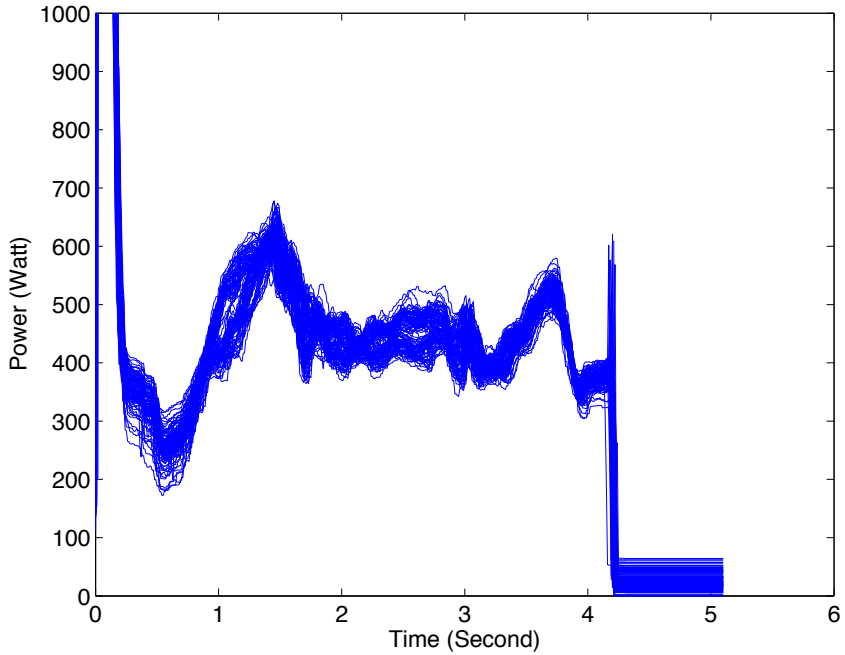
EM-MixRHLP clustering of simulated data





Clustering switch operations

Clustering real curves of switch operations The data set contains 115 curves of $R = 6$ operations electromechanical process
$K = 2$ clusters: operating state without/with possible defect



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Clustering real curves of switch operations The data set contains 115 curves of $R = 6$ operations electromechanical process
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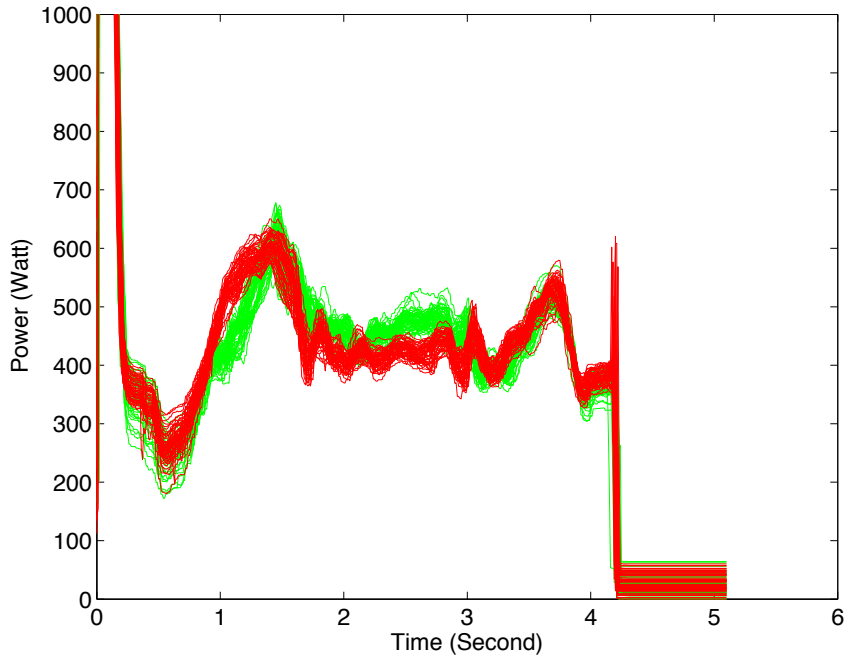


Functional discriminant analysis

Supervised classification context

- Data: a training set of labeled functions $((\boldsymbol{x}_1, \boldsymbol{y}_1, c_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{y}_n, c_n))$ where $c_i \in \{1, \ldots, G\}$ is the class label of the ith curve
- Problem: predict the class label c_i for a new unlabeled function $(\boldsymbol{x}_i, \boldsymbol{y}_i)$

Tool: Discriminant analysis

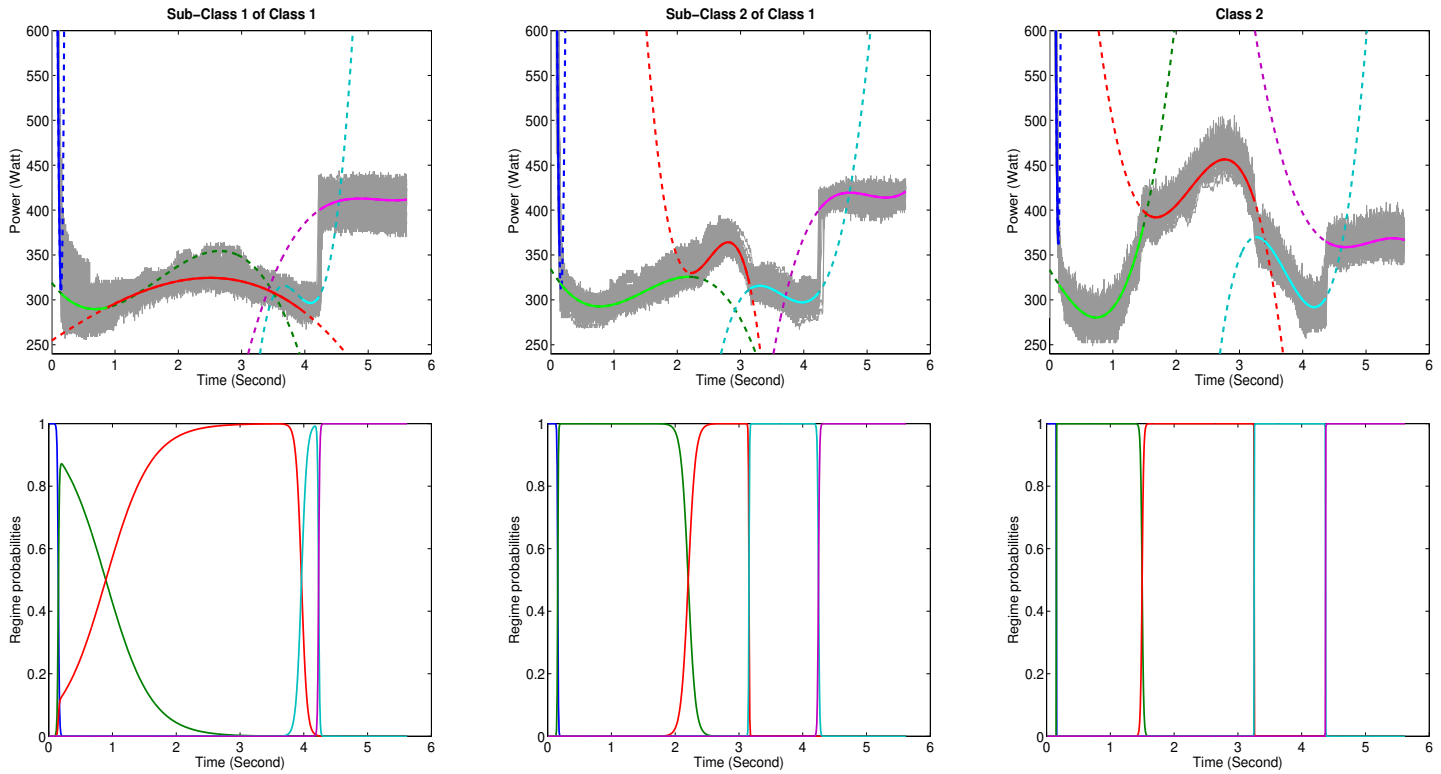
Use the Bayes' allocation rule

$$\hat{c}_i = \arg \max_{1 \leq g \leq G} \frac{\mathbb{P}(C_i = g) f(\boldsymbol{y}_i | \boldsymbol{x}_i; \boldsymbol{\Psi}_g)}{\sum_{g'=1}^{G} \mathbb{P}(C_i = g') f(\boldsymbol{y}_i | \boldsymbol{x}_i; \boldsymbol{\Psi}_{g'})},$$

based on a generative model $f(\boldsymbol{y}_i | \boldsymbol{x}_i; \boldsymbol{\Psi}_g)$ for each group g

- Homogeneous classes: Functional Linear Discriminant Analysis [8]
- Dispersed classes: Functional Mixture Discriminant Analysis [5]

Applications to switch curves



Approach	Classification error rate (%)	Intra-class inertia
FLDA-PR	11.5	10.7350×10^9
FLDA-SR	9.53	9.4503×10^9
FLDA-RHLP	8.62	8.7633×10^9
FMDA-PRM	9.02	7.9450×10^9
FMDA-SRM	8.50	5.8312×10^9
FMDA-MixRHLP	**6.25**	$\mathbf{3.2012 \times 10^9}$

Summary

- A full generative model for curve clustering and segmentation
- The segmentation is smoothly controlled by logistic functions
- An alternative to the previously described mixture of piecewise regressions
- more advantageous compared to approaches involving dynamic programming namely when using piecewise regression especially for large samples.
- Could be extended to the multivariate case without a major effort

Some ongoing research and perspectives

- Model-based co-clustering for high-dimensional functional data

Functional latent block model (FLBM) available soon on arXiv

Data: $\boldsymbol{Y} = (\boldsymbol{y}_{ij})$: n individuals defined on a set $\mathcal{I}$ with d continuous functional variables defined on a set $\mathcal{J}$ where $y_{ij}(t) = \mu(x_{ij}(t); \boldsymbol{\beta}) + \epsilon(t)$, t defined on$\mathcal{T}$.

- FLBM model:

$$
\begin{aligned}
f(\boldsymbol{Y}|\boldsymbol{X};\boldsymbol{\Psi}) &= \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \mathbb{P}(\mathbf{Z},\mathbf{W}) f(\boldsymbol{Y}|\boldsymbol{X},\mathbf{Z},\mathbf{W};\boldsymbol{\theta}) \\
&= \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \prod_{i,k} \pi_k^{z_{ik}} \prod_{j,\ell} \rho_\ell^{w_{j\ell}} \prod_{i,j,k,\ell} f(\boldsymbol{y}_{ij}|\boldsymbol{x}_{ij};\boldsymbol{\theta}_{k\ell})^{z_{ik}w_{j\ell}}.
\end{aligned}
$$

- An RHLP is used as a conditional block distribution $f(\boldsymbol{y}_{ij}|\boldsymbol{x}_{ij};\boldsymbol{\theta}_{k\ell})$
- Model inference using Stochastic EM

Some references

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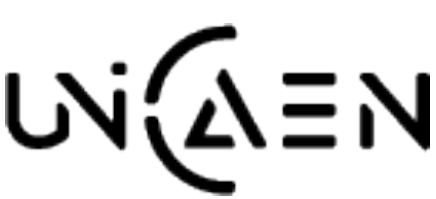
- F. Chamroukhi, A. Samé, G. Govaert, and P. Aknin. Time series modeling by a regression approach based on a latent process. *Neural Networks*, 22(5-6):593–602, 2009. URL `https://chamroukhi.users.lmno.cnrs.fr/papers/Chamroukhi_Neural_Networks_2009.pdf`

Unsupervised learning from high-dimensional and functional data

Faicel Chamroukhi

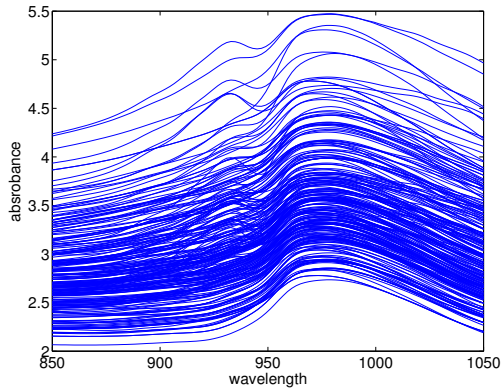



Research Summer School on Statistics for Data Science S4D 2018

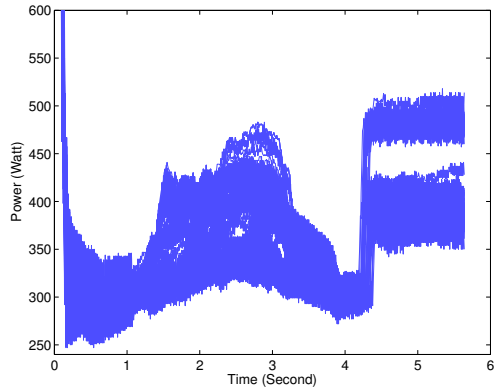
June 22, 2018

Functional data are increasingly frequent

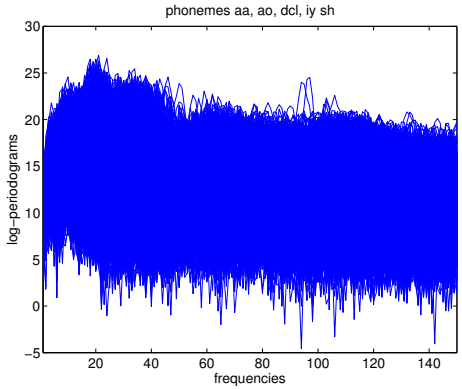
Chamroukhi and Nguyen [2018]



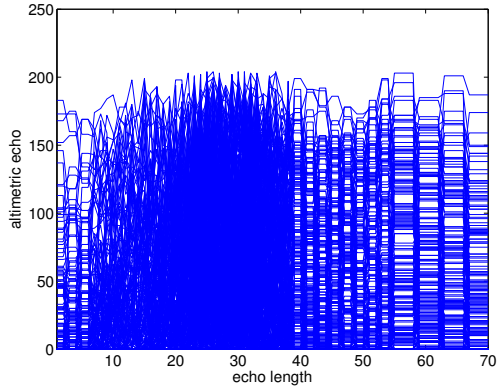
Tecator data



Railway switch curves



Phonemes curves



Satellite waveforms

Clustering of functional data

Tecator data set[1]: $n = 240$ spectra with $m = 100$ observations for each spectrum

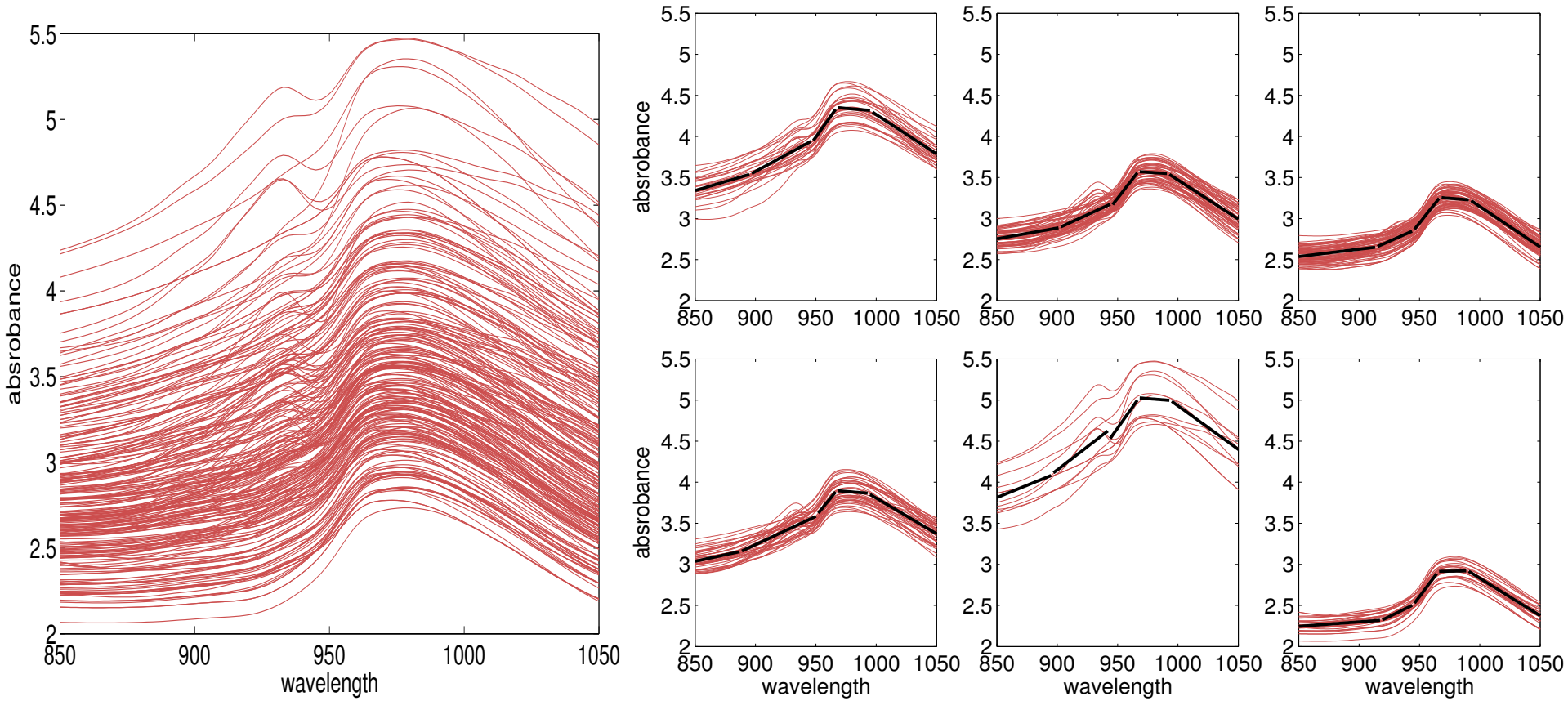


Figure: Original data and clustering results from Chamroukhi [2016] for the data considered in the same setting as in Hébrail et al. [2010] (six clusters, each cluster is approximated by five linear segments ($R = 5, p = 1$))

[1] Tecator data are available at `http://lib.stat.cmu.edu/datasets/tecator`.

Multivariate functional data are increasingly present

Measurements collected from different network elements (transceivers, cells, sites. . .)

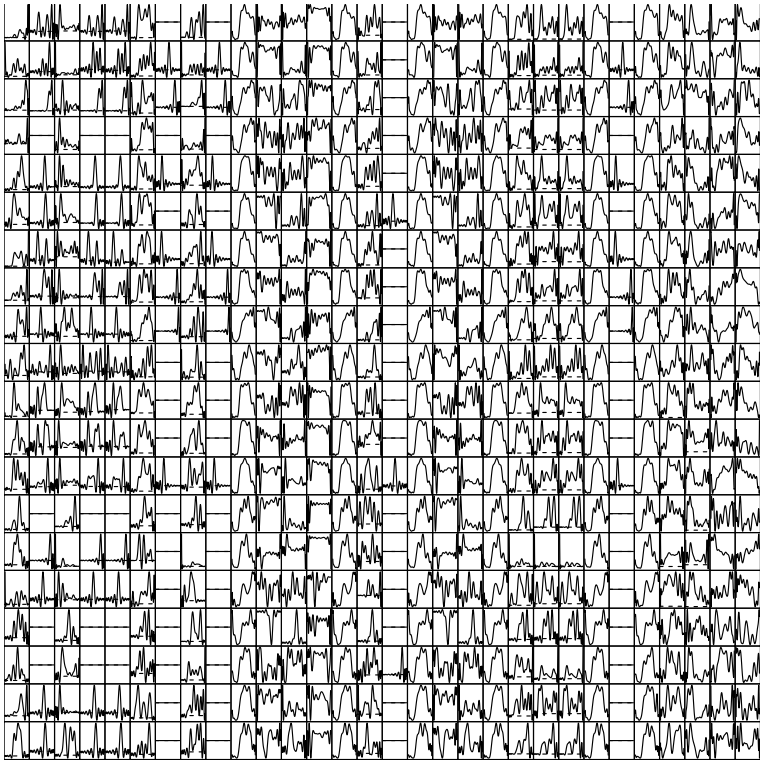


Figure: An example with $d = 30$ and $n = 20$ daily observations, from [Ben Slimen et al., 2016].

This talk

Questioning

Clustering of highly multivariate functional data with two guidelines:

- (1) Mathematical guideline: warranty for estimation and selection
- (2) User guideline: keep a user-friendly meaning of the process

Both are important because clustering is a highly risky task...

Proposed answering

(1) Model-based co-clustering with (2) temporal curve segmentation

Novelty corresponds to combining both (1) and (2)

Difference between clustering and co-clustering

- Simultaneous clustering of lines/indiv. ($\boldsymbol{Z}$) and columns/var. ($\boldsymbol{W}$)
- Can be used as a way to reduce dimensionality (var. $\rightarrow \boldsymbol{W}$)

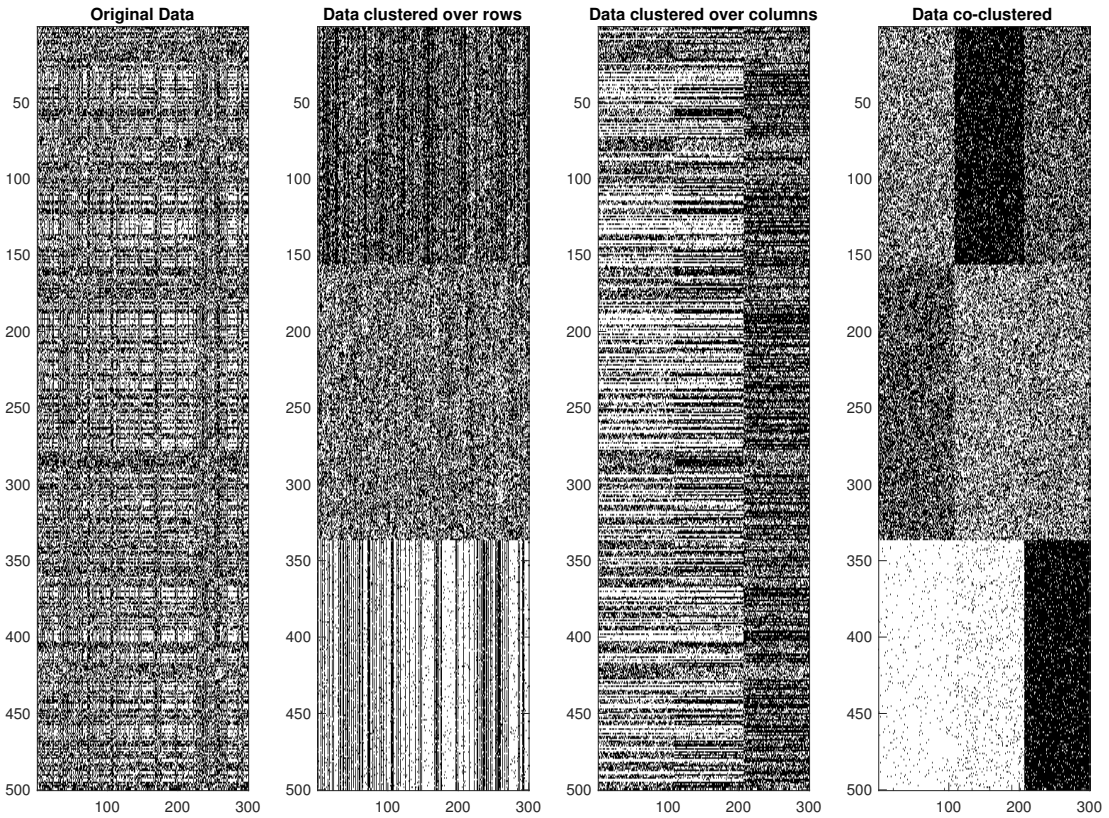


Figure: Binary data set with $n = 500$, $d = 300$, $K = M = 3$

Latent block model for co-clustering

$$f(\boldsymbol{X};\boldsymbol{\Psi}) \quad = \quad \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \mathbb{P}(\boldsymbol{Z},\boldsymbol{W};\boldsymbol{\pi},\boldsymbol{\rho}) \underbrace{f(\boldsymbol{X}|\boldsymbol{Z},\boldsymbol{W};\boldsymbol{\theta})}_{\text{data kind dependent}}$$

- The latent variables $\boldsymbol{Z}$ and $\boldsymbol{W}$ are independent: $\mathbb{P}(\boldsymbol{Z},\boldsymbol{W}) = \mathbb{P}(\boldsymbol{Z})\mathbb{P}(\boldsymbol{W})$ and iid:
  $\mathbb{P}(\boldsymbol{Z}) = \prod_i \mathbb{P}(z_i)$ with $z_i \sim$ Multinomial$(\pi_1,\ldots,\pi_K)$ where $\pi_k = \mathbb{P}(z_k = k)$
  $\mathbb{P}(\boldsymbol{W}) = \prod_j \mathbb{P}(w_j)$ with $w_j \sim$ Multinomial$(\rho_1,\ldots,\rho_M)$ where $\rho_\ell = \mathbb{P}(w_j = \ell)$
- Conditional independence: $x_{ij}|(z_i,w_j) \perp x_{i\prime j\prime}|(z_{i\prime},w_{j\prime})$

↪ binary data: binary [Govaert and Nadif, 2003, 2008; Keribin et al., 2012],
↪ categorical data: multinomial [Keribin et al., 2014]
↪ contingency table: Poisson [Govaert and Nadif, 2003, 2006, 2008]
↪ continuous data: Gaussian [Lomet, 2012; Govaert and Nadif, 2013]
↪ functional data: functional PCA + Gaussian, see further [Ben Slimen et al., 2016]

Inference for the latent block model

- Parameter estimation: maximum likelihood with variational block EM algorithm (VBEM) [Govaert and Nadif, 2006, 2008]
- Number of blocks estimation: ICL criterion

Recent or ongoing theoretical waranties for consistency

Functional data notation

- Data: (discretized) values of underlying smooth functions, not just vectors
- Data: A sample of n heterogeneous univariate curves $(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{y}_n)$
- $(\boldsymbol{x}_i, \boldsymbol{y}_i)$ consists of m_i observations $\boldsymbol{y}_i = (y_{i1}, \ldots, y_{im_i})$ observed at the independent covariates, (e.g., time t in time series), $(x_{i1}, \ldots, x_{im_i})$

Functional data modeling: "classical" approach

[Ramsay and Silverman, 2005] and many others

- Step 1: $(\boldsymbol{x}, \boldsymbol{y})$ decomposed into a finite basis of function (B-spline. . .)
- Step 2: functional principal components analysis (PCA) which is performed as a usual PCA of the basis expansion coefficients $\mathbf{c}$ using a metric defined by the inner products between the basis functions
- Step 3: set a distribution of probability on $\mathbf{c}$, typically Gaussian

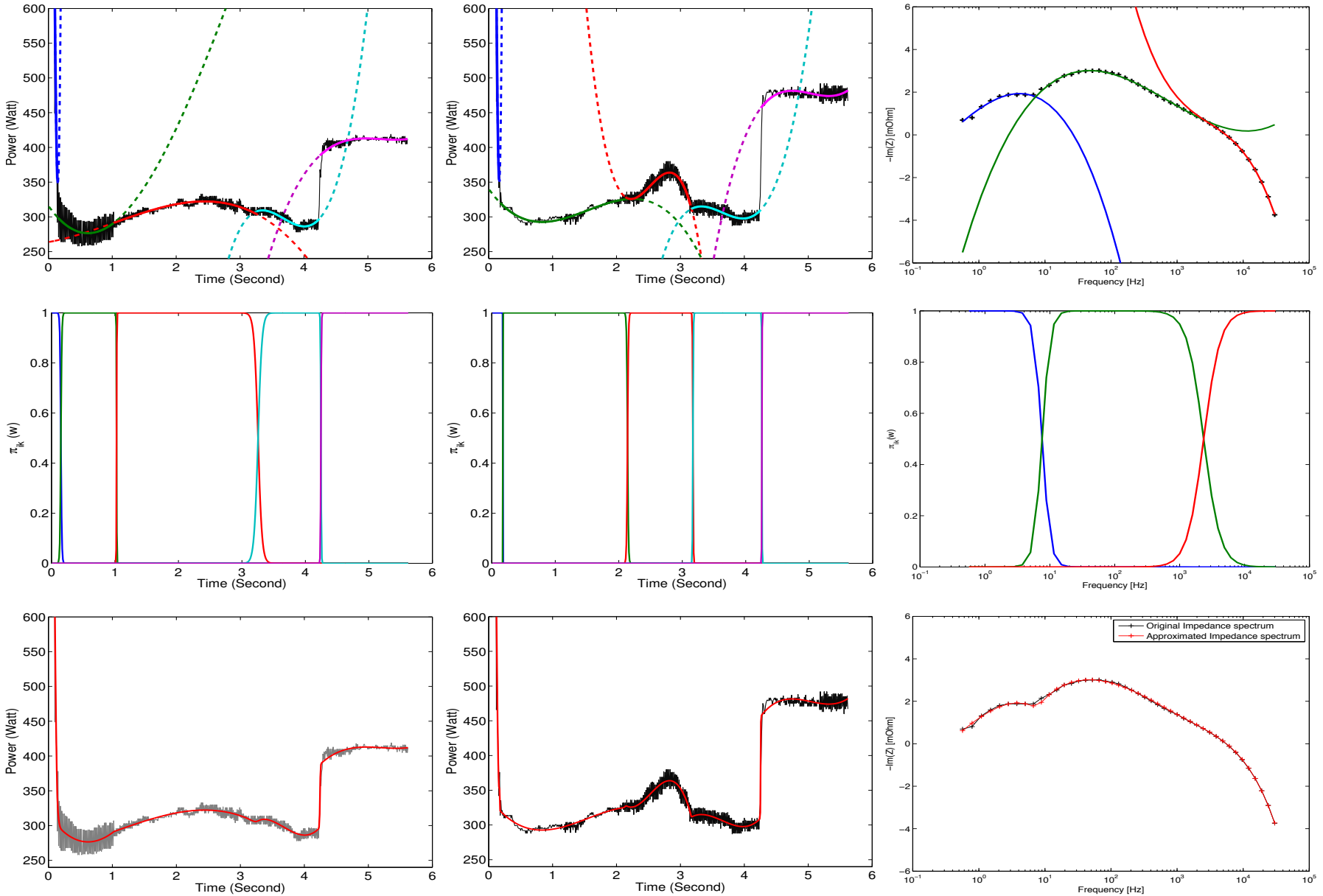
It defines a distribution on $\mathbf{c}$ instead of $\boldsymbol{y}$. . .

Functional data modeling: regression RHLP

Alternatively, use a segmentation via generative piecewise polynomial regression modeling of $f(\boldsymbol{y}|\boldsymbol{x})$ [Chamroukhi et al.])
$\hookrightarrow$ Regression with Hidden Logistic Process (RHLP)
$\hookrightarrow$ See formula later

It gives a distribution on $\boldsymbol{y}$ and also a meaningful segmentation of the curve

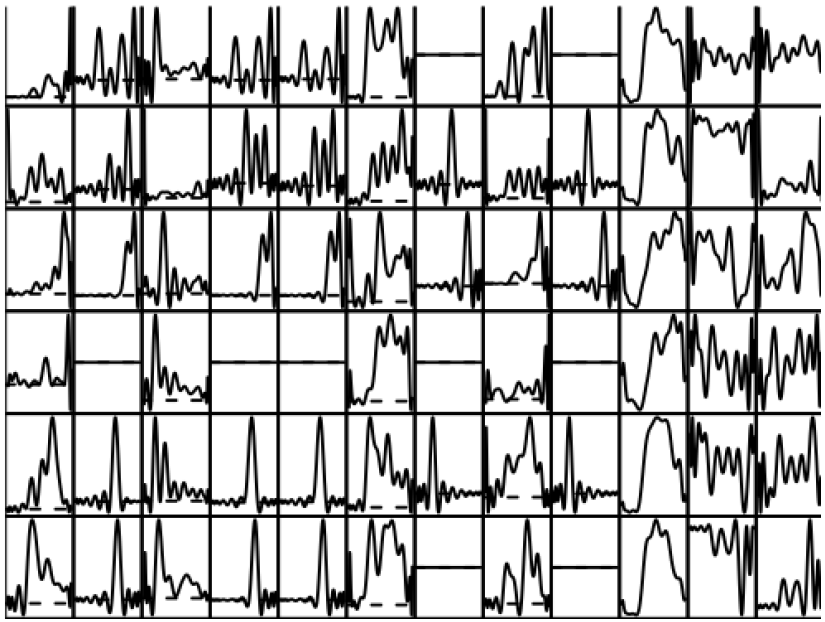
RHLP for modeling different kinds of functions



Multivariate functional data

Chamroukhi and Biernacki [2017]

- Data: $\boldsymbol{Y} = (\boldsymbol{y}_{ij})$ a data sample matrix of n individuals defined on a set $\mathcal{I}$ and d continuous functional variables defined on a set $\mathcal{J}$.
- Each variable $\boldsymbol{y}_{ij}$ is an univariate curve $\boldsymbol{y}_{ij} = \big(y_{ij}(t_1), \ldots, y_{ij}(t_{T_{ij}})\big)$ of T_{ij} observations $y(t) \in \mathbb{R}$ linked to covariates $\boldsymbol{x}_{ij} = \big(x_{ij}(t_1), \ldots, x_{ij}(t_{T_{ij}})\big)$ at the points $(t_1, \ldots, t_{T_{ij}})$, typically a sampling time



Embedding RHLP in co-clustering

Chamroukhi and Biernacki [2017]

- Co-clustering:

$$
\begin{aligned}
f(\boldsymbol{Y}|\boldsymbol{X};\boldsymbol{\Psi}) &= \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \mathbb{P}(\boldsymbol{Z};\boldsymbol{\pi})\mathbb{P}(\boldsymbol{W};\boldsymbol{\rho}) f(\boldsymbol{Y}|\boldsymbol{X},\boldsymbol{Z},\boldsymbol{W};\boldsymbol{\theta}) \\
&= \sum_{(z,w)\in\mathcal{Z}\times\mathcal{W}} \prod_{i,k} \pi_k^{z_{ik}} \prod_{j,\ell} \rho_\ell^{w_{j\ell}} \prod_{i,j,k,\ell} \underbrace{f(\boldsymbol{y}_{ij}|\boldsymbol{x}_{ij};\boldsymbol{\theta}_{k\ell})}_{\text{RHLP}}^{z_{ik}w_{j\ell}}.
\end{aligned}
$$

with parameter vector $\boldsymbol{\Psi} = (\boldsymbol{\pi}^T, \boldsymbol{\rho}^T, \boldsymbol{\theta}^T)^T$, where $\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K)^T$, $\boldsymbol{\rho} = (\rho_1, \ldots, \rho_M)^T$, and $\boldsymbol{\theta} = (\boldsymbol{\theta}_{11}^T, \ldots, \boldsymbol{\theta}_{k\ell}^T, \ldots, \boldsymbol{\theta}_{KM}^T)^T$.

Embedding RHLP in co-clustering

- RHLP: model the conditional data distribution for each block kl, assuming that each functional variable $\boldsymbol{y}_{ij}$ is governed by an $S_{k\ell}$-state hidden process of y_{ij}:

$$f(\boldsymbol{y}_{ij}|\boldsymbol{x}_{ij};\boldsymbol{\theta}_{k\ell}) = \prod_{t=1}^{T_{ij}} \sum_{r=1}^{S_{k\ell}} \alpha_{k\ell r}(t;\boldsymbol{\xi}_{k\ell}) \mathcal{N}\left(y_{ij}(t);\boldsymbol{\beta}_{k\ell r}^T \boldsymbol{x}_{ij}(t), \sigma_{k\ell r}^2\right)$$

where the dynamical weights α's are given by the multinomial logistic:

$$\alpha_{k\ell r}(t;\boldsymbol{\xi}_{k\ell}) = \frac{\exp\left(\xi_{k\ell r0} + \xi_{kr\ell 1} t\right)}{\sum_{r'=1}^{S_{k\ell}} \exp\left(\xi_{k\ell r'0} + \xi_{k\ell r'1} t\right)}.$$

$\hookrightarrow$ Can be seen as a generative piecewise polynomial regression model where the transition points are smoothly controlled by logistic weights

Parameter estimation: EM not feasible

- The complete-data log-likelihood:

$$\begin{aligned}\log L_c(\boldsymbol{\Psi}) &= \log f(\boldsymbol{Y}, \boldsymbol{Z}, \boldsymbol{W}, \boldsymbol{H}|\boldsymbol{X}; \boldsymbol{\Psi}) \\ &= \sum_{i,k} z_{ik} \log \pi_k + \sum_{j,\ell} w_{j\ell} \log \rho_\ell \\ &\quad + \sum_{i,j,k,\ell,t,r} z_{ik} w_{j\ell} h_{tr} \log \left[\alpha_{k\ell r}(t; \boldsymbol{\xi}_{k\ell}) \mathcal{N}\left(y_{ij}(t); \boldsymbol{\beta}_{k\ell r}^T \boldsymbol{x}_{ij}(t), \sigma_{k\ell r}^2 \right) \right]\end{aligned}$$

where $(h_{tr}; t = 1, \ldots, T_{ij}, r = 1, \ldots, S_{k\ell})$ is a binary variable indicating from which state the observation $y_{ij}(t)$ within the block cluster $k\ell$ is originated

Parameter estimation: EM not feasible

- The E-Step computes the expected complete-data log-likelihood, given the observed curves $(\boldsymbol{X}, \boldsymbol{Y})$, and the current parameter estimation $\boldsymbol{\Psi}^{(q)}$

$$
\begin{aligned}
Q(\boldsymbol{\Psi}, \boldsymbol{\Psi}^{(q)}) =& \mathbb{E}\left[\log L_c(\boldsymbol{\Psi}) \middle| \boldsymbol{X}, \boldsymbol{Y}; \boldsymbol{\Psi}^{(q)}\right] \\
=& \sum_{i,k} \mathbb{P}(z_{ik} = 1 | \boldsymbol{y}_{ij}, \boldsymbol{x}_{ij}) \log \pi_k + \sum_{j,\ell} \mathbb{P}(w_{j\ell} = 1 | \boldsymbol{y}_{ij}, \boldsymbol{x}_{ij}) \log \rho_\ell \\
&+ \sum_{i,j,k,\ell,t,r} \mathbb{P}(z_{ik} w_{j\ell} = 1 | \boldsymbol{y}_{ij}, \boldsymbol{x}_{ij}) \mathbb{P}(h_{tr} = 1 | z_{ik}, w_{j\ell}, y_{ij}(t), x_{ij}(t)) \times \\
&\log\left[\alpha_{k\ell r}(t; \boldsymbol{\xi}_{k\ell}) \mathcal{N}\left(y_{ij}(t); \boldsymbol{\beta}_{k\ell r}^T \boldsymbol{x}_{ij}(t), \sigma_{k\ell r}^2\right)\right]
\end{aligned}
$$

↪ Requires the calculation of the posterior joint distribution $\mathbb{P}(z_{ik} w_{j\ell} = 1 | \boldsymbol{y}_{ij}, \boldsymbol{x}_{ij})$

↪ does not factorize due to the conditional dependence on the observed curves of the row and the column labels

⇒ [Govaert and Nadif, 2008, 2013] proposed a variational approximation by relying on the Neal and Hinton's interpretation of the EM algorithm [Neal and Hinton, 1998].

↪ We adopt this variational approximation in our context

Variational block EM algorithm

$$\mathbb{P}(z_{ik}w_{j\ell}=1|\boldsymbol{y}_{ij},\boldsymbol{x}_{ij}) \approx \mathbb{P}(z_{ik}=1|\boldsymbol{y}_{ij},\boldsymbol{x}_{ij}) \times \mathbb{P}(w_{j\ell}=1|\boldsymbol{y}_{ij},\boldsymbol{x}_{ij})$$

Initialization: start from an initial solution at iteration $q=0$, and then alternate at the $(q+1)$th iteration between the following variational E- and M- steps until convergence:

VE Step Estimate the variational approximated posterior memberships:

1. $\tilde{z}_{ik}^{(q+1)} \propto$
   $\pi_k^{(q)} \exp\Big(\sum_{j,\ell,t,r} \tilde{w}_{j\ell}^{(q)}\ \tilde{h}_{tr}^{(q)} \log\Big[\alpha_{k\ell r}(t;\boldsymbol{\xi}_{k\ell}^{(q)})\mathcal{N}\left(y_{ij}(t);\boldsymbol{\beta}_{k\ell r}^{T(q)}\boldsymbol{x}_{ij}(t),\sigma_{k\ell r}^{(q)^2}\right)\Big]\Big)$
2. $\tilde{w}_{j\ell}^{(q+1)} \propto$
   $\rho_\ell^{(q)} \exp\Big(\sum_{i,k,t,r} \tilde{z}_{ik}^{(q)}\ \tilde{h}_{tr}^{(q)} \log\Big[\alpha_{k\ell r}(t;\boldsymbol{\xi}_{k\ell}^{(q)})\mathcal{N}\left(y_{ij}(t);\boldsymbol{\beta}_{k\ell r}^{T(q)}\boldsymbol{x}_{ij}(t),\sigma_{k\ell r}^{(q)^2}\right)\Big]\Big)$
3. $\tilde{h}_{tr}^{(q+1)} \propto \alpha_{k\ell r}^{(q)}(t;\boldsymbol{\xi}_{k\ell}^{(q)})\mathcal{N}\left(y_{ij}(t);\boldsymbol{\beta}_{k\ell r}^{(q)^T}\boldsymbol{x}_{ij}(t),\sigma_{k\ell r}^{(q)^2}\right)$

where: $\tilde{z}_{ik}=\mathbb{P}(z_{ik}=1|\boldsymbol{y}_{ij},\boldsymbol{x}_{ij})$, $\tilde{w}_{j\ell}=\mathbb{P}(w_{j\ell}=1|\boldsymbol{y}_{ij},\boldsymbol{x}_{ij})$,
$\tilde{h}_{tr}=\mathbb{P}(h_{tr}=1|z_i,w_j,y_{ij}(t),x_{ij}(t))$

Variational block EM algorithm

M Step update the parameters estimates $\boldsymbol{\theta}^{(q+1)}$ given the estimated posterior memberships at the current iteration $q+1$:

1. $\pi_k^{(q+1)} = \frac{\sum_i \tilde{z}_{ik}^{(q+1)}}{n}$
2. $\rho_\ell^{(q+1)} = \frac{\sum_j \tilde{w}_{j\ell}^{(q+1)}}{d}$

   The update of each block parameters $\boldsymbol{\theta}_{k\ell}$ consists in a weighted version of the RHLP updating rules:

3. $\boldsymbol{\xi}_{k\ell}^{(new)} = \boldsymbol{\xi}_{k\ell}^{(old)} - \left[\frac{\partial^2 F(\boldsymbol{\xi}_{k\ell})}{\partial \boldsymbol{\xi}_{k\ell} \partial \boldsymbol{\xi}_{k\ell}^T}\right]^{-1}_{\boldsymbol{\xi}_{k\ell}=\boldsymbol{\xi}_{k\ell}^{(old)}} \left.\frac{\partial F(\boldsymbol{\xi}_{k\ell})}{\partial \boldsymbol{\xi}_{k\ell}}\right|_{\boldsymbol{\xi}_{k\ell}=\boldsymbol{\xi}_{k\ell}^{(old)}}$ which is the IRLS maximisation of $F(\boldsymbol{\xi}_{k\ell}) = \sum_{i,j,t} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \tilde{h}_{tr}^{(q)} \log \alpha_{k\ell r}(t; \boldsymbol{\xi}_{k\ell})$ w.r.t $\boldsymbol{\xi}_{k\ell}$.

   The regression parameters updates consist in analytic WLS problems:

4. $\boldsymbol{\beta}_{k\ell r}^{(q+1)} = \left[\sum_{i,j} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \mathbf{X}_{ij}^T \boldsymbol{\Lambda}_{ijkr}^{(q)} \mathbf{X}_{ij}\right]^{-1} \sum_{i,j} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \mathbf{X}_{ij}^T \boldsymbol{\Lambda}_{ijkr}^{(q)} \boldsymbol{y}_{ij}$
5. $\sigma_{k\ell r}^{2(q+1)} = \frac{\sum_{i,j} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \| \sqrt{\boldsymbol{\Lambda}_{ijkr}^{(q)}} (\boldsymbol{y}_{ij} - \mathbf{X}_{ij} \boldsymbol{\beta}_{kr}^{(q+1)}) \|^2}{\sum_{i,j} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \ \text{trace}(\boldsymbol{\Lambda}_{ijkr}^{(q)})}$ where $\mathbf{X}_{ij}$ is the design matrix for the ith curve, $\boldsymbol{\Lambda}_{ijkr}^{(q)}$ is the diagonal matrix whose diagonal elements are the posterior segment memberships $\{\tilde{h}_{ijtr}^{(q)}; t = 1, \ldots, T_{ij}\}$.

Conclusion and perspectives

Conclusion

- A full generative framework for the cluster analysis and segmentation of high-dimensional non-stationary functional data
- The model inference can be performed by a variational EM algorithm

Perspectives

- Replace Variational EM by an SEM algorithm, which does not use approximation
- Numerical experiments
- Package

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Thank you for your attention!