SMILES

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FAICEL CHAMROUKHI

ANR-SMILES kickoff meeting, 14 feb 2019

SMILES (nov 2018, for 42 months)

Statistical Modeling and Inference for unsupervised Learning at LargE-Scale

Partners :

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Université de Rouen Normandie, LMRS	G. Chagny (resp.), A. Channarond, N. Vergne, C. Bérard, A. Roche
Université de Toulon, LIS Laboratoire d'Informatique & Systèmes	H. Glotin (resp.), S. Paris, J. Razik, R. Marxer
Inria informatics mathematics	C. Biernacki (resp.), V. Vandewalle

Context and Objectives

- **Context :** Large-scale data are increasingly frequent : Complex data $\hookrightarrow$ *heterogeneous, dynamical (temporal, functional), incomplete, high-dimension, and possibly massive*
- **Objectives :** learn/discern useful information in an unsupervised way from raw data :
  $\hookrightarrow$ Reconstruct/reveal hidden structures, i.e, (hierarchy of) groups ; learn/select relevant features, etc

General scientific framework

$\hookrightarrow$ Statistical **latent data models** (LDM) : $f(x|\boldsymbol{\theta}) = \int_{\mathcal{Z}} f(x, z|\boldsymbol{\theta}) \mathrm{d}z$, at scale (functional data, random graphs, acoustic data)

$\hookrightarrow$ **Unsupervised statistical inference** at large-scale (regularization, resampling, etc) : $\widehat{\boldsymbol{\theta}} \in \arg\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) - \mathrm{Pen}_{\lambda}(\boldsymbol{\theta})$

Research Axes

1. Task 1 : Models and inference for unsupervised large-scale data classification.
   - Sub-task 1.1 : Large-scale model-based clustering. (LMNO, INRIA) :
   - Sub-task 1.2 : Large-scale LDM and inference for functional data. (LMNO, INRIA) :
   - Sub-task 1.3 : Large-Scale LDM and inference for discrete data. (LMRS, LMNO, INRIA) :

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2. Task 2 : Models and inference for large-scale data representation.
   - Sub-task 2.1 : High-dimensional (non-)parametric sparse regression for large-scale representation (LMRS, LMNO) :
   - Sub-task 2.2 : Unsupervised large-scale multimodal data representation (LIS, LMNO) :

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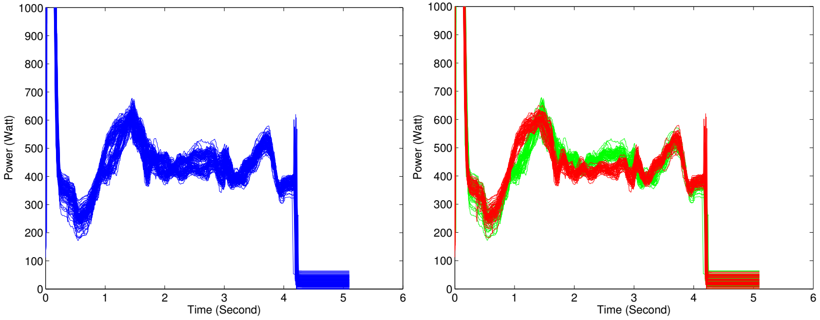
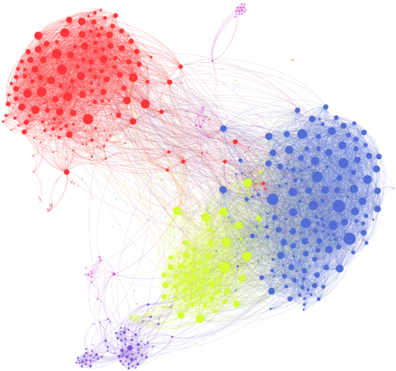
3. Task 3 : Validation and applications.
   - i) Large-scale functional data analysis (LMNO-INRIA-LMRS) of heterogeneous multivariate times series and fMRI images
   - ii) Large-scale Bioacoustical data analysis (LIS-LMNO) for environmental survey
   - iii) Large-scale biological data analysis (LMRS) by inferring large-scale biological sequences from high-throughput sequencing

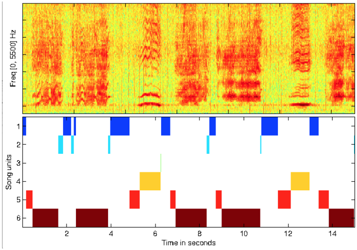
High-dimensional FDA by clustering/segmentation

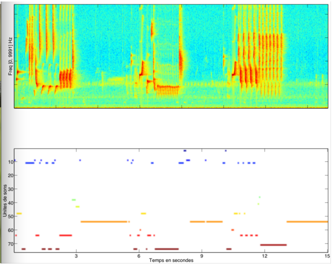


Large-scale graph clustering by latent-bloc models



Unsupervised Sparse Signal Decomposition





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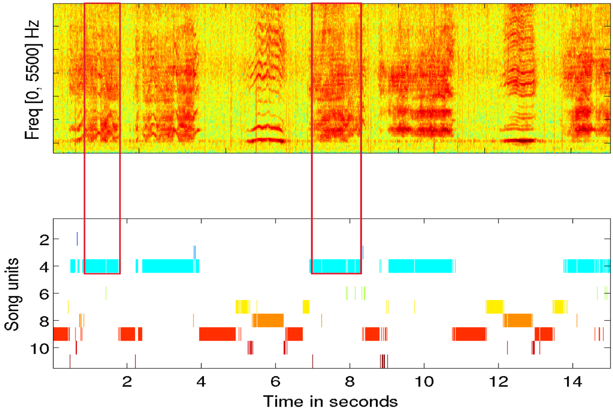
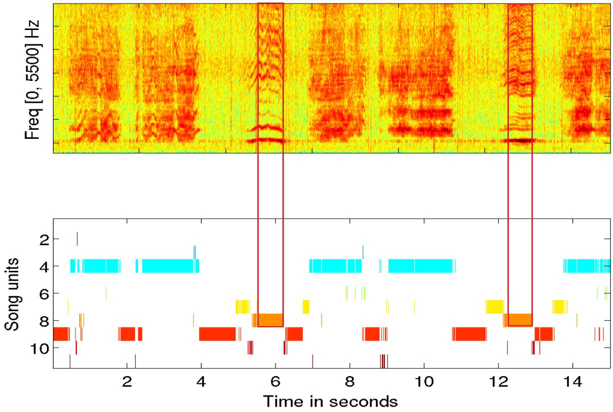


DÃ©composition parcimonieuse non-supervisÃ©e



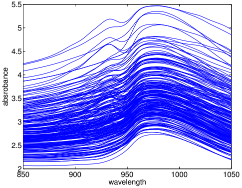
Outline

Model-Based Co-Clustering of Multivariate Functional Data
Joint work with Christophe Biernacki, INRIA-Lille

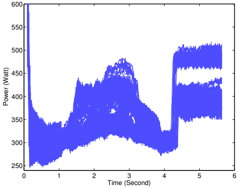
Outline

Functional data are increasingly frequent

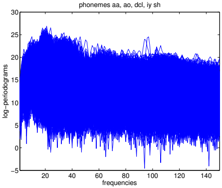
(James and Hastie, 2001; James and Sugar, 2003)
(Ramsay and Silverman, 2005)
(Chamroukhi et al., 2010)
(Bouveyron and Jacques, 2011)
(Samé et al., 2011)
(Jacques and Preda, 2014)
(Bouveyron et al., 2018)
(Chamroukhi and Nguyen, 2018)



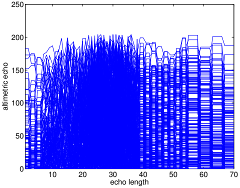
Tecator data



Railway switch curves



Phonemes curves



Satellite waveforms

Clustering of functional data

$\hookrightarrow$ a growing investigation of Model-Based Clustering (MBC) for functional data

Some Reviews on MBC for functional data : (Jacques and Preda, 2014; Chamroukhi and Nguyen, 2018)

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Tecator data set [1] : $n = 240$ spectra with $m = 10($

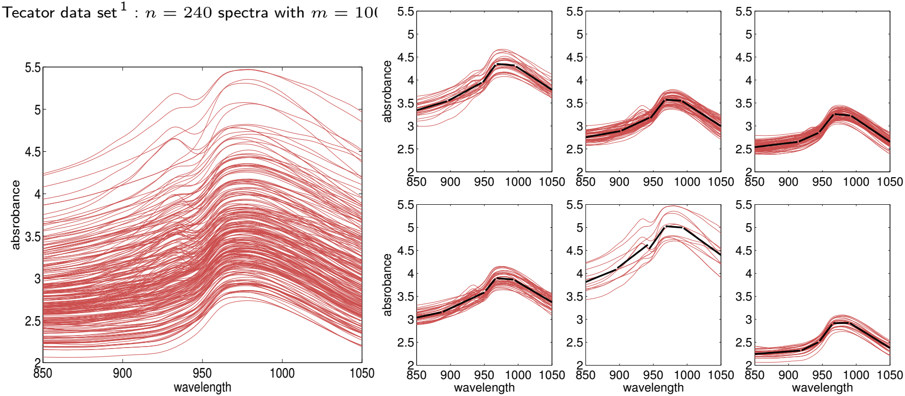


FIGURE – Original data and clustering results from Chamroukhi (2016) for the data considered in the same setting as in Hébrail et al. (2010) (six clusters, each cluster is approximated by five linear segments $(R = 5, p = 1)$)

Clustering of functional data

Topex/Poseidon satellite data [2] : $n = 472$ waveforms of $m = 70$ measured echoes

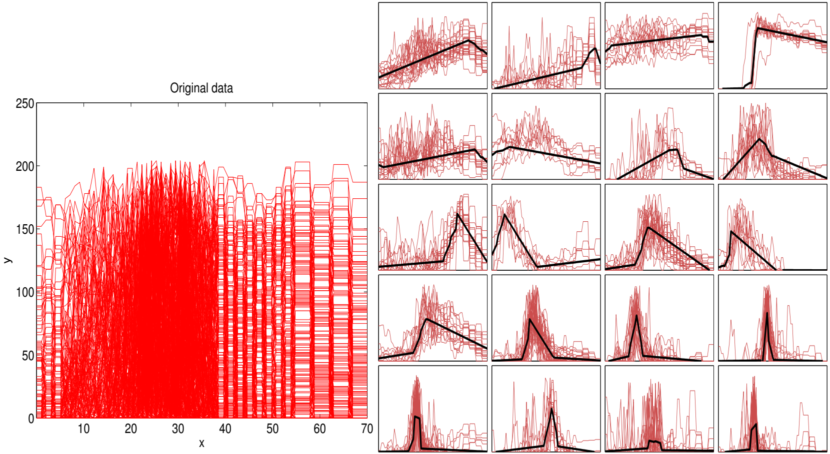


FIGURE – Original data and clustering results from Chamroukhi (2016) with the same setting as in Hébrail et al. (2010) : twenty clusters and a piecewise linear approximation of four segments.

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

Clustering of functional data

Phonemes data set [3] : $n = 1000$ log-periodograms for $m = 150$ frequencies

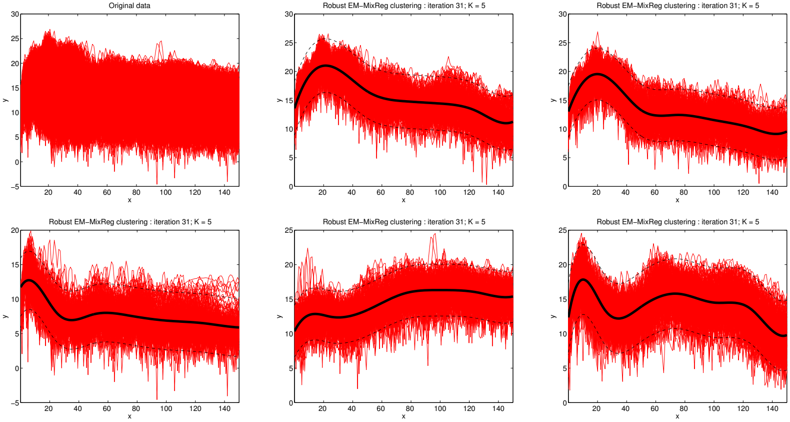


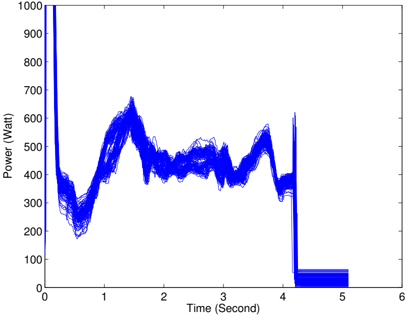
FIGURE – Original data and clustering results from Chamroukhi (2016)

3. Data from `http://www.math.univ-toulouse.fr/staph/npfda/`, used in Ferraty and Vieu (2003)

Clustering real curves of high-speed railway-switch operations

Data : $n = 115$ curves of $m \simeq 510$ observations

$K = 2$ clusters : operating state without/with possible defect



Clustering switch operations

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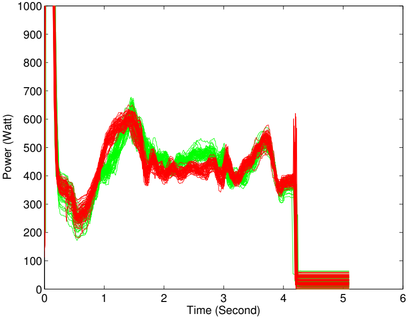


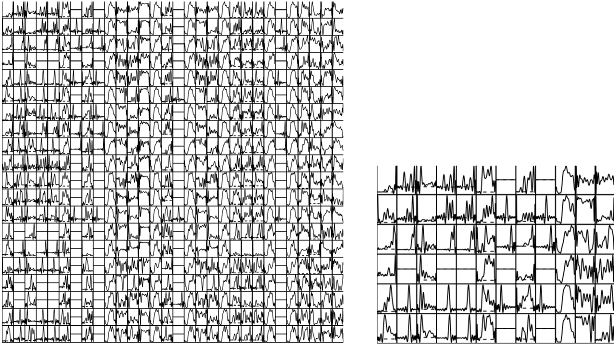
Outline

1. Model-Based Co-Clustering of Multivariate Functional Data
   - Motivation
   - Model-based co-clustering
   - Temporal curve segmentation (RHLP)
   - Model-based co-clustering embedding RHLP
   - Conclusion and perspectives

This talk : Multivariate functional data clustering

- Multivariate functional data are increasingly present
- e.g : Data continuously recorded for different subjects from multiple subject' sensors

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



Data Zoom

FIGURE – An example with $d = 30$ and $n = 20$ daily observations (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. $\rightarrow \boldsymbol{W}$)

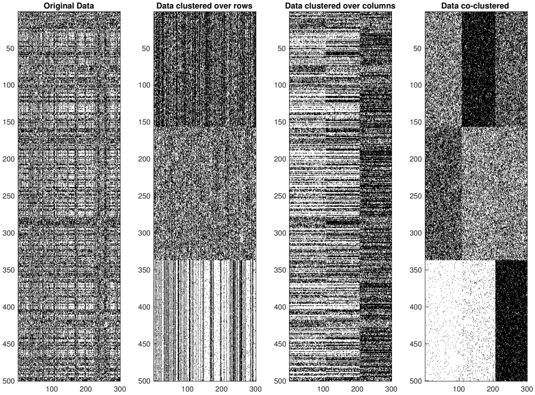


FIGURE – Binary data set with $n = 500$, $d = 300$, $K = M = 3$

Latent block model for co-clustering

The Latent Block Model (Govaert and Nadif, 2013)

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

Hypotheses

- 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 : $x_{ij}|(z_i,w_j) \perp x_{i'j'}|(z_{i'},w_{j'})$

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$\hookrightarrow$ binary data : binary (Govaert and Nadif, 2003, 2008; Keribin et al., 2012),

$\hookrightarrow$ categorical data : multinomial (Keribin et al., 2014)

$\hookrightarrow$ contingency table : Poisson (Govaert and Nadif, 2003, 2006, 2008)

$\hookrightarrow$ continuous data : Gaussian (Lomet, 2012; Govaert and Nadif, 2013)

$\hookrightarrow$ functional data : functional PCA + Gaussian, see further (Ben Slimen et al., 2016)

Inference for the latent block model

Inference of the latent block model

- variational block EM (VBEM) for maximum likelihood estimation and fuzzy co-clustering (Govaert and Nadif, 2006, 2008).
- block classification EM (CEM) algorithm for maximum classification likelihood and hard co-clustering (Govaert and Nadif, 2003, 2006, 2008)
- Bayesian inference (Keribin et al., 2012, 2014) : Bayesian latent block mixtures for binary data and categorical data & a variational Bayesian inference and Gibbs sampling.
- Number of blocks estimation : ICL criterion (Lomet, 2012; Keribin et al., 2014)

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. . .) : $Y_i(t) \approx \sum_{r=1}^{d} c_{ir}\phi_r(x_i(t))$ with $\mathbf{c}$ estimated by OLS
- 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 probability distribution on $\mathbf{c}$, typically Gaussian

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

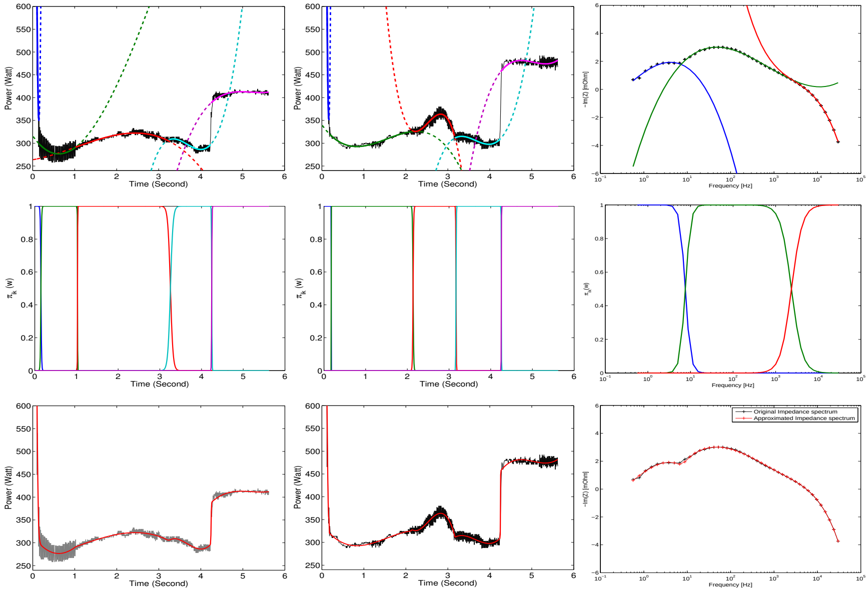
Functional data modeling : regression RHLP

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

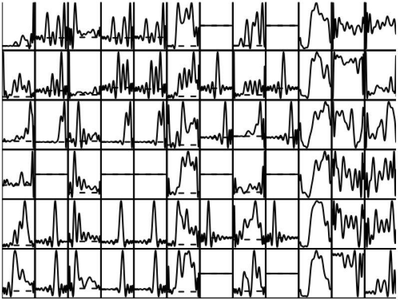
RHLP for modeling different types of functions



Multivariate functional data co-clustering

(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)

- Functional Latent Block Model for 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 (Chamroukhi et al., 2009) : 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 :

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

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

$\hookrightarrow$ a particular mixture-of-experts model (Jacobs et al., 1991; Jordan and Jacobs, 1994)/(parametric) mixture of regressions with predictor-dependent mixing proportions (Young and Hunter, 2010)

Block mean curve approximation and segmentation

- Approximation : a prototype mean curve

$$y_t|(z_i, w_j) \approx \widehat{y}_t = \mathbb{E}[Y(t)|z_i, w_j, x(t); \widehat{\boldsymbol{\Psi}}] = \sum_{s=1}^{S_{kl}} \alpha_{k\ell r}(t; \widehat{\boldsymbol{\xi}}_{k\ell}) \widehat{\boldsymbol{\beta}}_{k\ell r}^T \boldsymbol{x}_i(t)$$

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

- Curve segmentation :

$$\widehat{h}_t|(z_i, w_j) = \arg \max_{1 \leq s \leq S_{kl}} \mathbb{E}[H_t|z_i, w_j, x_{ij}(t); \widehat{\boldsymbol{\xi}}] = \arg \max_{1 \leq k \leq K} \alpha_{k\ell r}(t; \widehat{\boldsymbol{\xi}}_{k\ell})$$

Parameter estimation : EM not feasible

EM algorithm :

$$\boldsymbol{\Psi}^{(q+1)} \in \arg\max_{\boldsymbol{\Psi}} \mathbb{E}\left[\log L_c(\boldsymbol{\Psi})|\mathcal{D}, \boldsymbol{\Psi}^{(q)}\right]$$

- 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

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

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. $\rho_\ell^{(q+1)} = \frac{\sum_j \tilde{w}_{j\ell}^{(q+1)}}{d}$

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. $\boldsymbol{\xi}_{k\ell}^{(new)} = \boldsymbol{\xi}_{k\ell}^{(old)} - \left[\frac{\partial^2 F(\boldsymbol{\xi}_{k\ell})}{\partial \boldsymbol{\xi}_{k\ell} \partial \boldsymbol{\xi}_{k\ell}^T}\right]^{-1}_{\boldsymbol{\xi}_{k\ell}=\boldsymbol{\xi}_{k\ell}^{(old)}} \frac{\partial F(\boldsymbol{\xi}_{k\ell})}{\partial \boldsymbol{\xi}_{k\ell}}\Big|_{\boldsymbol{\xi}_{k\ell}=\boldsymbol{\xi}_{k\ell}^{(old)}}$ 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 $\boldsymbol{\xi}_{k\ell}$.

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. $\pi_k^{(q+1)} = \frac{\sum_i \tilde{z}_{ik}^{(q+1)}}{n}$
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   The update of each block parameters $\boldsymbol{\theta}_{k\ell}$ consists in a weighted version of the RHLP updating rules :

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   The regression parameters updates consist in analytic WLS problems :

4. $\boldsymbol{\beta}_{k\ell r}^{(q+1)} = \Big[\sum_{i,j} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \mathbf{X}_{ij}^T \boldsymbol{\Lambda}_{ijkr}^{(q)} \mathbf{X}_{ij}\Big]^{-1} \sum_{i,j} \tilde{z}_{ik}^{(q)} \tilde{w}_{j\ell}^{(q)} \mathbf{X}_{ij}^T \boldsymbol{\Lambda}_{ijkr}^{(q)} \boldsymbol{y}_{ij}$
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 $\{\tilde{h}_{ijtr}^{(q)}; t = 1, \ldots, T_{ij}\}$.

$\hookrightarrow$ It is also possible to use the Classification EM (CEM) approximation of EM (Celeux and Govaert, 1992).

Parameter estimation by an SEM algorithm : SEM-FLBM

- $\hookrightarrow$ The SEM algorithm (Celeux and Diebolt, 1985) allows to overcome some drawbacks of the variational-EM algorithm, including its sensitivity to starting values ; SEM does not use an approximation.
- Eg. SEM for latent block models for categorical data (Keribin et al., 2012, 2014)
- The formulas of VEM-FLBM and SEM-FLBM are essentially the same, except that we incorporate a stochastic step consisting of sampling binary indicator variables z_{ik}, $w_{j\ell}$ and h_{tr} according to $\tilde{z}_{ik}$, $\tilde{w}_{j\ell}$ and $\tilde{h}_{tr}$.

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 or SEM

Perspectives

- Numerical experiments
- Package

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Thank you for your attention !