

A hidden process regression model for functional data description. Application to curve discrimination

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ABSTRACT

A new approach for functional data description is proposed in this paper. It consists of a regression model with a discrete hidden logistic process which is adapted for modeling curves with abrupt or smooth regime changes. The model parameters are estimated in a maximum likelihood framework through a dedicated expectation maximization (EM) algorithm. From the proposed generative model, a curve discrimination rule is derived using the maximum a posteriori rule. The proposed model is evaluated using simulated curves and real world curves acquired during railway switch operations, by performing comparisons with the piecewise regression approach in terms of curve modeling and classification.

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1. Introduction

Curve valued or functional data sets are increasingly available in science, engineering and economics. The work presented in this paper relates to the diagnosis of the French railway switches (or points) which enable trains to be guided from one track to another at a railway junction. The switch is controlled by an electrical motor and the considered curves are the condition measurements acquired during switch operations. Each curve represents the electrical power consumed during a switch operation (see Fig. 1).

To achieve the diagnosis task, the acquired curves have to be accurately summarized. Summarizing these curves can be performed by finding a simplified representation of each class of curves using an adapted model.

The switch operations curves can be seen as functional data presenting non-linearities and different changes in regime due to the mechanical motions involved in a switch operation (see Fig. 1). In this context, basic polynomial regression models cannot be used to find an accurate description of such data. An alternative approach consists in using splines to approximate each set of curves [15,14] but this requires the setting of knots. Another approach, that allows for fitting several (polynomial) models to the curves for different time ranges, consists in the piecewise polynomial regression model used in [19,2,8,13] for

curve approximation and segmentation. A related segmentation method is the segmentation-clustering approach of Picard et al. [21] applied to array CGH data. One can also distinguish the recently proposed algorithm of Hugueney et al. [13] for curves clustering and segmentation using piecewise regression.

Let's recall that piecewise polynomial regression is a representation and segmentation method that partitions curves into K segments (or regimes), each segment being characterized by its mean polynomial curve and its variance. The parameters estimation is performed using Fisher's algorithm [9] which globally optimizes an additive cost function [18] using a dynamic programming procedure [1]. The piecewise regression model is more adapted for modeling curves presenting abrupt changes and is less efficient for curves including regimes with smooth transitions. Moreover, the dynamic programming procedure is computationally expensive, especially for large samples.

In this paper, a generative model is explored to give a synthetic representation of a set of curves presenting changes in regime. The basic idea of the proposed model is to fit a specific regression model incorporating a discrete hidden process allowing for abrupt or smooth transitions between different polynomial regression models. This approach is an extension, to a set of curves, of the works presented in [5,4]. It is related to the switching regression model introduced in [22] and is very linked to the mixture of experts (ME) model [16,28] by the using of a time-dependent logistic transition function.

In addition to providing a simplified representation of functional data, the proposed model can be used for curve discrimination through the maximum a posteriori (MAP) rule. A related method is the functional linear discriminant analysis (FLDA) [15], where a cubic spline is used for curves approximation. More details about the functional data analysis (FDA)

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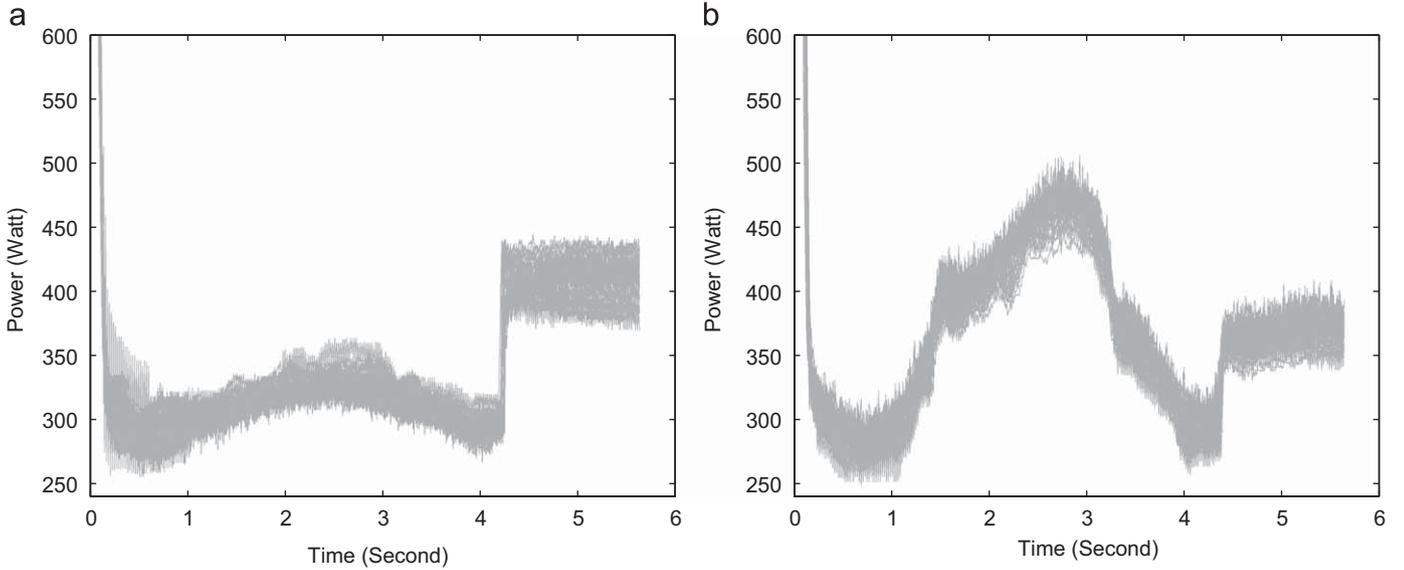


Fig. 1. Examples of curves of electrical power consumed during various switch operations: 35 curves correspond to operations without defect (a) and 45 curves correspond to operation with critical defect (b).

framework can be found in [23,24]. Other works for curve classification include neural network approaches [26] and kernel-based learning methods [25].

This paper is organized as follows. Section 2 provides an account of the piecewise polynomial regression model in the context of modeling a set of curves and the used parameter estimation technique based on dynamic programming. Section 3 introduces the proposed model for functional data representation and provides details of the parameters estimation by means of a dedicated EM algorithm. The curves approximation with the proposed approach is then presented and a curve classification scheme using the MAP rule is used. Section 4 deals with the experimental study carried out on simulated curves and real switch operation curves to assess the proposed approach.

2. Modeling a set of curves by the piecewise polynomial regression model

This section provides an overview of the piecewise polynomial regression model in a context of curves description and briefly recalls the algorithm used to estimate its parameters.

The piecewise polynomial regression is a segmentation method that partitions the data into K segments (or regimes). Generally used to model a single curve or time series [19,2,8,5], the piecewise polynomial regression model can be used to model a set of curves [13]. The parameters estimation is performed using a dynamic programming procedure [1,9,18] due to the additivity of the optimized cost function over the K segments.

Let \mathcal{X} be a training set of n curves $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ where each curve \mathbf{x}_i consists of m measurements (x_{i1}, \dots, x_{im}) observed at the time points (t_1, \dots, t_m) . In the following, the term “curves size” will be used to define m . The piecewise regression model assumes that the curves \mathcal{X} incorporate K polynomial regimes defined on K intervals whose bounds indexes can be denoted by $\gamma = (\gamma_1, \dots, \gamma_{K+1})$ with $\gamma_1 = 0$ and $\gamma_{K+1} = m$. This defines a partition of \mathcal{X} into K segments of curves $\{\mathbf{X}_1, \dots, \mathbf{X}_K\}$ of lengths m_1, \dots, m_K , respectively, where $\mathbf{X}_k = (\mathbf{x}_1^k, \dots, \mathbf{x}_n^k)^T$ is the $nm_k \times 1$ vector of the elements in the k th segment for the n curves with $\mathbf{x}_i^k = \{x_{ij} | j \in I_k\}$ is the set of elements in segment k of the i th curve whose indexes are $I_k = (\gamma_k, \gamma_{k+1}]$. Therefore, for each curve \mathbf{x}_i ($i = 1, \dots, n$), the piecewise polynomial regression model can be

defined as follows:

$$\forall j = 1, \dots, m, \quad x_{ij} = \beta_k^T \mathbf{r}_j + \sigma_k \varepsilon_{ij}, \quad \varepsilon_{ij} \sim \mathcal{N}(0, 1), \quad (1)$$

where k satisfies $j \in I_k$, β_k is the $p+1$ dimensional coefficients vector of a p degree polynomial associated with the k th segment with $k \in \{1, \dots, K\}$, $\mathbf{r}_j = (1, t_j, t_j^2, \dots, t_j^p)^T$ is the time dependent $p+1$ dimensional covariate vector associated with β_k . As in classical regression models, the ε_{ij} are assumed to be independent random variables distributed according to a standard Gaussian distribution representing the additive noise.

The model parameters can be denoted by (ψ, γ) where $\psi = (\beta_1, \dots, \beta_K, \sigma_1^2, \dots, \sigma_K^2)$ is the set of polynomial coefficients and noise variances, and $\gamma = (\gamma_1, \dots, \gamma_{K+1})$ is the set of the transition points.

2.1. Maximum likelihood estimation for the piecewise polynomial regression model

The estimation of the parameter vector (ψ, γ) is performed by maximum likelihood. As in classical model-based learning problems where each observation is described by a feature vector [11], we assume that the curves sample $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is independent. Within a segment I_k , the independence of the noises ε_{ij} ($j \in I_k$) involves the independence of x_{ij} ($j \in I_k$) conditionally on t_j ($j \in I_k$). Thus, according to model (1), it can be proved that the observation x_{ij} , given the segment k , has a Gaussian distribution with mean $\beta_k^T \mathbf{r}_j$ and variance σ_k^2 . Therefore, the distribution of a curve \mathbf{x}_i is given by

$$p(\mathbf{x}_i; \psi, \gamma) = \prod_{k=1}^K \prod_{j \in I_k} \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2), \quad (2)$$

and the log-likelihood of the parameter vector (ψ, γ) characterizing the piecewise regression model, given the curves sample $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is then written as follows:

$$\begin{aligned} L(\psi, \gamma; \mathcal{X}) &= \sum_{k=1}^K \sum_{i=1}^n \sum_{j \in I_k} \log \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2) \\ &= -\frac{1}{2} \sum_{k=1}^K \left[\frac{1}{\sigma_k^2} \sum_{i=1}^n \sum_{j \in I_k} (x_{ij} - \beta_k^T \mathbf{r}_j)^2 + nm_k \log \sigma_k^2 \right] - \frac{nm}{2} \log 2\pi, \end{aligned} \quad (3)$$

where m_k is the cardinal number of I_k .

Maximizing this log-likelihood is equivalent to minimizing, with respect to ψ and γ , the criterion

$$J(\psi, \gamma) = \sum_{k=1}^K \left[\frac{1}{\sigma_k^2} \sum_{i=1}^n \sum_{j \in I_k} (x_{ij} - \hat{\beta}_k^T \mathbf{r}_j)^2 + nm_k \log \sigma_k^2 \right]. \quad (4)$$

The next section shows how the parameters ψ and γ can be estimated using the dynamic programming.

2.2. Parameter estimation for the piecewise regression model by the Fisher algorithm

Fisher algorithm is based on a dynamic programming procedure that provides the optimal segmentation of the data by minimizing an additive criterion [9,18,2]. It can be used to minimize (4) with respect to ψ and γ or equivalently to minimize (5) with respect to γ :

$$C(\gamma) = \min_{\psi} J(\psi, \gamma) = \sum_{k=1}^K \min_{(\beta_k, \sigma_k^2)} \left[\frac{1}{\sigma_k^2} \sum_{i=1}^n \sum_{j=\gamma_k+1}^{\gamma_{k+1}} (x_{ij} - \hat{\beta}_k^T \mathbf{r}_j)^2 + nm_k \log \sigma_k^2 \right] \\ = \sum_{k=1}^K \left[\frac{1}{\hat{\sigma}_k^2} \sum_{i=1}^n \sum_{j=\gamma_k+1}^{\gamma_{k+1}} (x_{ij} - \hat{\beta}_k^T \mathbf{r}_j)^2 + nm_k \log \hat{\sigma}_k^2 \right], \quad (5)$$

with

$$\hat{\beta}_k = \arg \min_{\beta_k} \sum_{i=1}^n \sum_{j=\gamma_k+1}^{\gamma_{k+1}} (x_{ij} - \beta_k^T \mathbf{r}_j)^2 = (\mathbf{M}_k^T \mathbf{M}_k)^{-1} \mathbf{M}_k^T \mathbf{X}_k, \quad (6)$$

and

$$\hat{\sigma}_k^2 = \frac{1}{nm_k} \sum_{i=1}^n \sum_{j=\gamma_k+1}^{\gamma_{k+1}} (x_{ij} - \hat{\beta}_k^T \mathbf{r}_j)^2, \quad (7)$$

where

$$\mathbf{M}_k = \begin{bmatrix} \Phi_k \\ \vdots \\ \Phi_k \end{bmatrix}$$

is the $nm_k \times (p+1)$ regression matrix of the segment k for all the curves and

$$\Phi_k = \begin{bmatrix} 1 & t_{\gamma_k+1} & t_{\gamma_k+1}^2 & \cdots & t_{\gamma_k+1}^p \\ 1 & t_{\gamma_k+2} & t_{\gamma_k+2}^2 & \cdots & t_{\gamma_k+2}^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & t_{\gamma_{k+1}} & t_{\gamma_{k+1}}^2 & \cdots & t_{\gamma_{k+1}}^p \end{bmatrix}$$

is the $m_k \times (p+1)$ regression matrix for the segment k for each curve.

We can see that the criterion $C(\gamma)$ is the sum of the cost $1/\hat{\sigma}_k^2 \sum_{i=1}^n \sum_{j=\gamma_k+1}^{\gamma_{k+1}} (x_{ij} - \hat{\beta}_k^T \mathbf{r}_j)^2 + nm_k \log \hat{\sigma}_k^2$ over the K segments. The additivity of this criterion means it can be optimized globally using a dynamic programming procedure [1,18]. Dynamic programming considers that an optimal partition of the data into K segments is the union of an optimal partition into $K-1$ segments and one segment. Thus, by denoting by $C_1(a,b)$ the optimal cost within one segment whose elements indexes are (a,b) with $0 \leq a < b \leq m$, the optimal costs $C_k(a,b)$ for a partition into k segments, $k=2, \dots, K$, is recursively computed

as follows:

$$\begin{cases} C_1(a,b) = \min_{(\beta, \sigma^2)} \left[\frac{1}{\sigma^2} \sum_{i=1}^n \sum_{j=a+1}^b (x_{ij} - \beta^T \mathbf{r}_j)^2 + n(b-a) \log \sigma^2 \right] \\ = \frac{1}{\hat{\sigma}^2} \sum_{i=1}^n \sum_{j=a+1}^b (x_{ij} - \hat{\beta}^T \mathbf{r}_j)^2 + n(b-a) \log \hat{\sigma}^2, \\ C_k(a,b) = \min_{a \leq h \leq b} [C_{k-1}(a,h) + C_1(h+1,b)] \quad \text{for } k=2, \dots, K, \end{cases} \quad (8)$$

where $\hat{\beta}$ and $\hat{\sigma}^2$ are computed, respectively, according to the Eqs. (6) and (7) by replacing (γ_k, γ_{k+1}) by (a,b) , m_k by $(b-a)$ and $\hat{\beta}_k$ by $\hat{\beta}$. Thus, the algorithm works as follows:

Step 1: Initialization.

This step consists of computing the cost matrix $C_1(a,b)$ for one segment (a,b) for $0 \leq a < b \leq m$ using (8).

Step 2: Dynamic programming procedure.

This step consists of recursively computing the optimal cost $C_k(a,b)$ for $k=2, \dots, K$ and $0 \leq a < b \leq m$ using (8).

Step 3: Finding the optimal partition.

The optimal partition can be deduced from the optimal costs $C_k(a,b)$. (For more details see Appendix A of [2]).

This algorithm has a time complexity of $\mathcal{O}(Kp^2n^2m^2)$ which can be computationally expensive for large sample sizes.

2.3. Curves approximation and classification with the piecewise regression model

2.3.1. Curves approximation

Once the model parameters are estimated, the curves approximation derived from the piecewise polynomial regression model is given by $\hat{x}_{ij} = \sum_{k=1}^K \hat{z}_{jk} \hat{\beta}_k^T \mathbf{r}_j$, $\forall i=1, \dots, n$, $\forall j=1, \dots, m$ where $\hat{z}_{jk} = 1$ if $j \in (\hat{\gamma}_k, \hat{\gamma}_{k+1}]$ and $\hat{z}_{jk} = 0$ otherwise. The vectorial formulation of the curves approximation $\hat{\mathcal{X}}$ can be written as

$$\hat{\mathcal{X}} = \sum_{k=1}^K \hat{Z}_k \mathbf{T} \hat{\beta}_k, \quad (9)$$

where \hat{Z}_k is a diagonal matrix whose diagonal elements are $(\hat{z}_{1k}, \dots, \hat{z}_{mk})$, and

$$\mathbf{T} = \begin{bmatrix} 1 & t_1 & t_1^2 & \cdots & t_1^p \\ 1 & t_2 & t_2^2 & \cdots & t_2^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & t_m & t_m^2 & \cdots & t_m^p \end{bmatrix}$$

is the $m \times (p+1)$ regression matrix.

2.3.2. Curve classification

This section presents the discrimination rule which can be derived from the piecewise polynomial regression approach to classify curves into predefined classes.

Let us denote by C_i the class label of the curve \mathbf{x}_i , which takes its values in the finite set $\{1, \dots, G\}$ where G is the number of classes. Given a labeled training set of curves, the parameter vectors $(\hat{\psi}_1, \hat{\gamma}_1), \dots, (\hat{\psi}_G, \hat{\gamma}_G)$ for the G classes are estimated by the dynamic programming procedure. Once the classes parameters are estimated, a new acquired curve \mathbf{x}_i is assigned to the class \hat{g} that maximizes the posterior probability that \mathbf{x}_i belongs to the class g , ($g=1, \dots, G$):

$$\hat{g} = \arg \max_{1 \leq g \leq G} p(C_i = g | \mathbf{x}_i; \hat{\psi}_g, \hat{\gamma}_g), \quad (10)$$

where

$$p(C_i = g | \mathbf{x}_i; \hat{\psi}_g, \hat{\gamma}_g) = \frac{p(C_i = g)p(\mathbf{x}_i | C_i = g; \hat{\psi}_g, \hat{\gamma}_g)}{\sum_{g'=1}^G p(C_i = g')p(\mathbf{x}_i | C_i = g'; \hat{\psi}_{g'}, \hat{\gamma}_{g'})}, \quad (11)$$

$p(C_i = g)$ being the proportion of the class g in the training database and $p(\mathbf{x}_i | C_i = g; \hat{\psi}_g, \hat{\gamma}_g)$ the conditional density of \mathbf{x}_i given the class g defined by Eq. (2). The parameters $(\hat{\psi}_g, \hat{\gamma}_g)$ represent the maximum likelihood estimates of (ψ_g, γ_g) .

3. The proposed regression model with a hidden logistic process

Although the piecewise regression model described in the previous section is based on the global optimization of a likelihood criterion, it is naturally tailored for curves presenting abrupt changes since the obtained curve segmentation is hard. Moreover, it is well known that the dynamical programming procedure is computationally expensive for large sample sizes. This section presents the proposed regression model based on a hidden logistic process for functional data modeling. The flexibility of this model allows for modeling of curves with abrupt or smooth changes in regime.

3.1. The global regression model

In the proposed model, each curve \mathbf{x}_i from the set $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is assumed to be generated by the following regression model with a discrete hidden process $\mathbf{z} = (z_1, \dots, z_m)$:

$$\forall j = 1, \dots, m, \quad x_{ij} = \beta_{z_j}^T \mathbf{r}_j + \sigma_{z_j} \varepsilon_{ij}, \quad \varepsilon_{ij} \sim \mathcal{N}(0, 1), \quad (12)$$

where $z_j \in \{1, \dots, K\}$ is a hidden discrete variable representing the label of the polynomial regression model generating x_{ij} . This model can be reformulated in a matrix form by

$$\mathbf{x}_i = \sum_{k=1}^K Z_k(\mathbf{T}\beta_k + \sigma_k \varepsilon_i), \quad \varepsilon_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_m), \quad (13)$$

where Z_k is the $m \times m$ diagonal matrix whose diagonal elements are (z_{1k}, \dots, z_{mk}) , with $z_{jk} = 1$ if $z_j = k$ (i.e. if x_{ij} is generated by the k th regression model) and $z_{jk} = 0$ otherwise. The variable $\varepsilon_i = (\varepsilon_{i1}, \dots, \varepsilon_{im})^T$ is a $m \times 1$ noise vector distributed according to a Gaussian density with zero mean and identity covariance matrix.

The next section defines the probability distribution of the process $\mathbf{z} = (z_1, \dots, z_m)$ that allows the switching from one regression model to another.

3.2. The hidden logistic process

The proposed hidden logistic process assumes that the variables z_j ($j = 1, \dots, m$), given the vector $\mathbf{t} = (t_1, \dots, t_m)$, are generated independently according to the multinomial distribution $\mathcal{M}(1, \pi_{j1}(\mathbf{w}), \dots, \pi_{jK}(\mathbf{w}))$, where

$$\pi_{jk}(\mathbf{w}) = p(z_j = k; \mathbf{w}) = \frac{\exp(\mathbf{w}_{k0} + \mathbf{w}_{k1} t_j)}{\sum_{\ell=1}^K \exp(\mathbf{w}_{\ell 0} + \mathbf{w}_{\ell 1} t_j)}, \quad (14)$$

is the logistic transformation of a linear function of the time point t_j , $\mathbf{w}_k = (\mathbf{w}_{k0}, \mathbf{w}_{k1})^T$ is the two dimensional coefficients vector for the k th component of (14) and $\mathbf{w} = (\mathbf{w}_1, \dots, \mathbf{w}_K)$. Thus, given the

vector $\mathbf{t} = (t_1, \dots, t_m)$, the distribution of \mathbf{z} can be written as

$$p(\mathbf{z}; \mathbf{w}) = \prod_{j=1}^m \prod_{k=1}^K \left(\frac{\exp(\mathbf{w}_{k0} + \mathbf{w}_{k1} t_j)}{\sum_{\ell=1}^K \exp(\mathbf{w}_{\ell 0} + \mathbf{w}_{\ell 1} t_j)} \right)^{z_{jk}}. \quad (15)$$

The relevance of the logistic transformation in terms of flexibility of transition can be illustrated through simple examples with $K=2$ components. In this case, only the probability $\pi_{j1}(\mathbf{w}) = \exp(\mathbf{w}_{10} + \mathbf{w}_{11} t_j) / (1 + \exp(\mathbf{w}_{10} + \mathbf{w}_{11} t_j))$ should be described, since $\pi_{j2}(\mathbf{w}) = 1 - \pi_{j1}(\mathbf{w})$. The variation of the proportions $\pi_{jk}(\mathbf{w})$ over time, in relation to the parameter \mathbf{w}_k , is illustrated by an example of 2 classes where we use the parametrization $\mathbf{w}_k = \lambda_k(\alpha_k, 1)^T$, with $\lambda_k = \mathbf{w}_{k1}$ and $\alpha_k = \mathbf{w}_{k0} / \mathbf{w}_{k1}$.

As shown in Fig. 2(a), the parameter λ_k controls the quality of transitions between the regression models, the higher absolute value of λ_k , the more abrupt the transition between the z_j , while the parameter α_k controls the transition time point via the inflexion point of the curve (see Fig. 2(b)).

In this particular regression model, the variable z_j controls the switching from one regression model to another of K regression models within the curves at each time t_j . The use of the logistic process for modeling the sequence of variables z_j allows for modeling both abrupt and smooth transitions between the regimes within the curves, unlike the piecewise regression model which is adapted only for regimes with abrupt transitions.

3.3. The generative model of curves

The generative model of n curves from a fixed parameters $(\mathbf{w}, \beta_k, \sigma_k^2)$ for $k = 1, \dots, K$ consists of two steps:

- generate the hidden process $\mathbf{z} = (z_1, \dots, z_m)$ according to the multinomial distribution $z_j \sim \mathcal{M}(1, \pi_{j1}(\mathbf{w}), \dots, \pi_{jK}(\mathbf{w}))$,
- for $i = 1, \dots, n$ and for $j = 1, \dots, m$: generate each observation x_{ij} according to the Gaussian distribution $\mathcal{N}(\cdot; \beta_{z_j}^T \mathbf{r}_j, \sigma_{z_j}^2)$.

3.4. Parameter estimation

From the model (12), it can be proved that, conditionally on a regression model k , x_{ij} is distributed according to a normal density with mean $\beta_k^T \mathbf{r}_j$ and variance σ_k^2 . Thus, it can be proved that x_{ij} is distributed according to the normal mixture density

$$p(x_{ij}; \theta) = \sum_{k=1}^K \pi_{jk}(\mathbf{w}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2), \quad (16)$$

where $\theta = (\mathbf{w}, \beta_1, \dots, \beta_K, \sigma_1^2, \dots, \sigma_K^2)$ is the parameter vector to be estimated. The parameter θ is estimated by the maximum likelihood method.

As in the piecewise polynomial regression model, we assume that the curves sample $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is independent. The independence of the ε_{ij} 's ($j = 1, \dots, m$) involves the independence of the x_{ij} 's ($j = 1, \dots, m$) conditionally on the time vector $\mathbf{t} = (t_1, \dots, t_m)$. It should be noticed that the temporal dependence between the underlying segments is controlled by the logistic distribution. The distribution of \mathbf{x}_i is then written as

$$p(\mathbf{x}_i; \theta) = \prod_{j=1}^m \sum_{k=1}^K \pi_{jk}(\mathbf{w}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2). \quad (17)$$

Therefore, the log-likelihood of θ is written as

$$L(\theta; \mathcal{X}) = \log p(\mathbf{x}_1, \dots, \mathbf{x}_n; \theta) = \sum_{i=1}^n \sum_{j=1}^m \log \sum_{k=1}^K \pi_{jk}(\mathbf{w}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2). \quad (18)$$

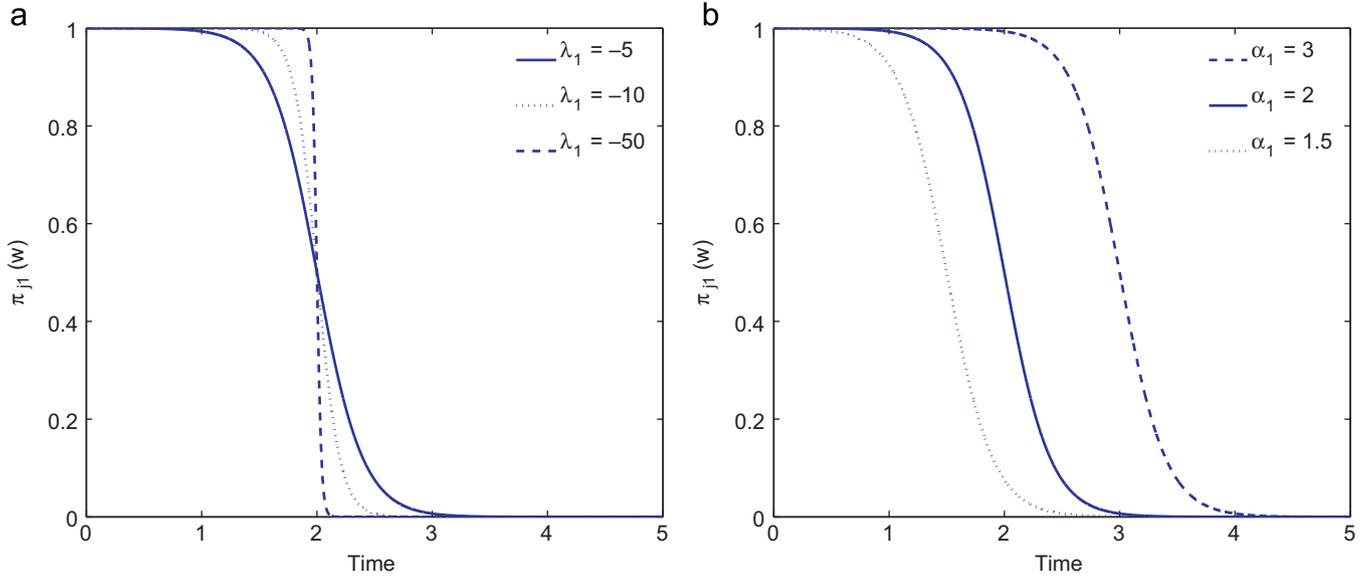


Fig. 2. Variation of $\pi_{j_1}(\mathbf{w})$ over time for a dimension $q=1$ of \mathbf{w}_1 and (a) different values of $\lambda_1 = \mathbf{w}_{11}$ with $\alpha_1 = -2$ and (b) different values of $\alpha_1 = \mathbf{w}_{10}/\mathbf{w}_{11}$ with $\lambda_1 = -5$.

The direct maximization of this likelihood is not straightforward, we use a dedicated expectation maximization (EM) algorithm [7,20] to perform the maximization.

3.5. The dedicated EM algorithm

The proposed EM algorithm starts from an initial parameter $\theta^{(0)}$ and alternates the two following steps until convergence.

E step (expectation): This step consists in computing the expectation of the complete log-likelihood $CL(\theta; \mathcal{X}, \mathbf{z}) = \log p(\mathcal{X}, \mathbf{z}; \theta)$ given the observed data \mathcal{X} and the current value $\theta^{(q)}$ of the parameter θ (q being the current iteration):

$$Q(\theta, \theta^{(q)}) = E[CL(\theta; \mathcal{X}, \mathbf{z}) | \mathcal{X}; \theta^{(q)}]. \quad (19)$$

This step simply requires the computation of the posterior probabilities

$$\tau_{ijk}^{(q)} = p(z_{jk} = 1 | x_{ij}; \theta^{(q)}) = \frac{\pi_{jk}(\mathbf{w}^{(q)}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2)}{\sum_{\ell=1}^K \pi_{j\ell}(\mathbf{w}^{(q)}) \mathcal{N}(x_{ij}; \beta_\ell^T \mathbf{r}_j, \sigma_\ell^2)} \quad (20)$$

that x_{ij} originates from the k th regression model (see appendix for details).

M step (maximization): In this step, the value of the parameter θ is updated by computing the parameter $\theta^{(q+1)}$ maximizing the conditional expectation Q with respect to θ .

Maximizing Q with respect to β_k ($k=1, \dots, K$) consists in analytically solving a weighted least-squares problem. The estimates are given by

$$\beta_k^{(q+1)} = (A^T W_k^{(q)} A)^{-1} A^T W_k^{(q)} \mathcal{X}, \quad (21)$$

where $W_k^{(q)}$ is the $nm \times nm$ diagonal matrix whose diagonal elements are the posterior probabilities $(\tau_{11k}^{(q)}, \dots, \tau_{1mk}^{(q)}, \dots, \tau_{n1k}^{(q)}, \dots, \tau_{nmk}^{(q)})$ for the k th regression component and A is the $nm \times (p+1)$ regression matrix for all the curves \mathcal{X} such that:

$$A = \begin{bmatrix} \mathbf{T} \\ \vdots \\ \mathbf{T} \end{bmatrix} \quad \text{and} \quad \mathcal{X} = \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}.$$

Maximizing Q with respect to σ_k^2 ($k=1, \dots, K$) provides the following updating formula:

$$\sigma_k^{2(q+1)} = \frac{1}{nm_k^{(q)}} \sum_{i=1}^n \sum_{j=1}^m \tau_{ijk}^{(q)} (x_{ij} - \beta_k^T \mathbf{r}_j)^2, \quad (22)$$

where $m_k^{(q)} = \sum_{j=1}^m \tau_{ijk}^{(q)}$ can be seen as the cardinal number of the component k estimated at iteration q for each curve \mathbf{x}_i (see appendix for more details).

The maximization of Q with respect to \mathbf{w} is a multinomial logistic regression problem weighted by $\tau_{ijk}^{(q)}$ which can be solved using a multi-class Iterative Reweighted Least Squares (IRLS) algorithm [10,6,17,4].

The proposed algorithm is performed with a time complexity of $\mathcal{O}(NMnmK^3p^2)$, where N is the number of iterations of the EM algorithm and M is the average number of iterations required by the IRLS algorithm used in the maximization step at each iteration of the EM algorithm. Thus, the ratio between the time complexity of the piecewise polynomial regression model and the time complexity of the proposed regression model is nm/NMK^2 . In practice, as illustrated in the computing time graphics (see Fig. 8), nm is larger than NMK^2 since the number of regimes K does not exceed 5 and a particular strategy is used to initialize the IRLS algorithm. This initialization consists in choosing an arbitrary value of the parameter \mathbf{w} only for the first iteration of the EM algorithm. For the other EM iterations, the IRLS loop starts with the parameter $\mathbf{w}^{(q)}$ estimated at the q th iteration of the EM algorithm and provides $\mathbf{w}^{(q+1)}$. This setting reduces the running time of the IRLS algorithm and thus reduces the running time of the EM algorithm.

3.6. Model selection

The optimal values of the pairs (K, p) can be computed by using the Bayesian Information Criterion (BIC) [27] which is a penalized likelihood criterion, defined by

$$\text{BIC}(K, p) = L(\hat{\theta}; \mathcal{X}) - \frac{v(K, p) \log(nm)}{2}, \quad (23)$$

where $v(K, p) = K(p+4) - 2$ is the number of parameters of the model and $L(\hat{\theta}; \mathcal{X})$ is the log-likelihood obtained at convergence of the EM algorithm.

3.7. Curves approximation and classification with the proposed model

3.7.1. Curves approximation

With the proposed description approach, the set of curves belonging to the same class is approximated by a single curve. Each point of this curve is given by the expectation $E(x_{ij}; \hat{\theta}) \forall i = 1, \dots, n$ and $\forall j = 1, \dots, m$ where

$$E(x_{ij}; \hat{\theta}) = \int_{\mathbb{R}} x_{ij} p(x_{ij}; \hat{\theta}) dx_{ij} = \sum_{k=1}^K \pi_{jk}(\hat{\mathbf{w}}) \int_{\mathbb{R}} x_{ij} \mathcal{N}(x_{ij}; \hat{\beta}_k^T \mathbf{r}_j, \hat{\sigma}_k^2) dx_{ij} = \sum_{k=1}^K \pi_{jk}(\hat{\mathbf{w}}) \hat{\beta}_k^T \mathbf{r}_j, \quad (24)$$

$\hat{\theta} = (\hat{\mathbf{w}}, \hat{\beta}_1, \dots, \hat{\beta}_K, \hat{\sigma}_1^2, \dots, \hat{\sigma}_K^2)$ being the parameter vector obtained at convergence of the algorithm. The matrix formulation of the curves approximation $\hat{\mathcal{X}}$ is given by:

$$\hat{\mathcal{X}} = \sum_{k=1}^K \hat{\lambda}_k \mathbf{T} \hat{\beta}_k, \quad (25)$$

where $\hat{\lambda}$ is a diagonal matrix whose diagonal elements are the proportions $(\pi_{1k}(\hat{\mathbf{w}}), \dots, \pi_{mk}(\hat{\mathbf{w}}))$ associated with the k th regression model.

3.7.2. Curve classification

Basing on the proposed curves modeling approach, a curve discrimination rule can be derived. Given a labeled training set of curves, the parameters $\theta_1, \dots, \theta_G$ of the G classes are first estimated by applying the proposed description approach to each class of curves. This approach is generally used for supervised learning of generative models. Whereas, for the discriminative approaches, which directly estimate the decision boundaries, the parameters of each class are not estimated independently from the other classes.

Once the classes parameters are estimated by the EM algorithm, a new acquired curve \mathbf{x}_i is assigned to the class \hat{g} , as described in Section 2.3.2, by the MAP rule:

$$\hat{g} = \arg \max_{1 \leq g \leq G} p(C_i = g | \mathbf{x}_i; \hat{\theta}_g), \quad (26)$$

where

$$p(C_i = g | \mathbf{x}_i; \hat{\theta}_g) = \frac{p(C_i = g) p(\mathbf{x}_i | C_i = g; \hat{\theta}_g)}{\sum_{g'=1}^G p(C_i = g') p(\mathbf{x}_i | C_i = g'; \hat{\theta}_{g'})}, \quad (27)$$

$p(\mathbf{x}_i | C_i = g; \hat{\theta}_g)$ being the conditional density of \mathbf{x}_i given the class g defined by Eq. (17). The parameter vector $\hat{\theta}_g = (\hat{\mathbf{w}}_g, \hat{\beta}_{1g}, \dots, \hat{\beta}_{K_g}, \hat{\sigma}_{1g}^2, \dots, \hat{\sigma}_{K_g}^2)$ is the maximum likelihood estimate of θ for the class g .

4. Experimental study

This section is devoted to an evaluation of the proposed approach in terms of curves description and classification, using simulated data sets and real data sets. For this purpose, the

proposed approach was compared with the piecewise polynomial regression approach. Two evaluation criteria were used.

- The first criterion is the mean square error between the true simulated curve without noise and the estimated curve given by
 - $\hat{x}_{ij} = \sum_{k=1}^K \pi_{jk}(\hat{\mathbf{w}}) \hat{\beta}_k^T \mathbf{r}_j$ for the proposed model;
 - $\hat{x}_{ij} = \sum_{k=1}^K \hat{z}_{jk} \hat{\beta}_k^T \mathbf{r}_j$ for the piecewise polynomial regression model.
 The mean square error criterion is computed by the formula $1/nm \sum_{i=1}^n \sum_{j=1}^m [E(x_{ij}; \theta) - \hat{x}_{ij}]^2$, θ being the true parameter vector. It is used to assess the models with regard to curves modeling.
- The second criterion is the curves misclassification error rate computed by a 5-fold cross-validation procedure.

4.1. Evaluation in terms of curves modeling

Three experiments were performed to evaluate the proposed approach in terms of curves modeling:

- the first experiment aims at observing the effect of the smoothness level of transitions on estimation quality. The smoothness level of transitions was tuned by means of the term $\lambda_k = \mathbf{w}_{k1}$ seen in Section 3.2 and Fig. 2(a). Each simulated sample of curves consisted of $n=10$ curves with a curves size $m=100$. The simulated curves consisted of three constant polynomial ($K=3, p=0$) with transition time points at 1 and 3 s. Each simulated curve consisted in a mean curve corrupted by an additive uniform zero-mean Gaussian noise with a standard deviation $\sigma = 2$. The j th point of the mean curve is given by $\sum_{k=1}^K \pi_{jk}(\mathbf{w}) \beta_k^T \mathbf{r}_j$. The set of simulation parameters $\{\beta_k, \mathbf{w}_k\}$ for this experiment is given in Table 1. We have considered decreasing values of $|\lambda_k|$, which correspond to increasing values of the smoothness level of transitions (see Table 2). Fig. 3(a) shows the true denoised curves for the 10 smoothness levels of transitions and Fig. 3(b) shows an example of simulated curves for a fixed smoothness level,
- the second experiment aims at observing the effect of the sample size n on estimation quality. It varies from 10 to 100 by step of 10, and the curves size was set to $m=100$,
- the third experiment aims at observing the effect of the curves size m on estimation quality. It varied from 100 to 1000 by step of 100 for a fixed number of curves $n=50$.

For the second and the third experiments, the curves were simulated with the proposed regression model with hidden logistic process given by Eq. (12). The simulated curves consisted of three polynomial regimes ($K=3$) with a polynomial of order $p=2$ with transition time points at 1 and 4 s. Table 3 shows the set of simulation parameters for these experiments and Fig. 4 shows an example of simulated curves with $n=50$ and $m=100$. For all the experiments, we considered that the curves were observed over 5 s with a constant sampling period ($\Delta t = t_j - t_{j-1}$ is constant).

Table 1
Simulation parameters for experiment 1.

$\beta_1 = 0$	$\mathbf{w}_1 = [3341.33, -1706.96]$
$\beta_2 = 10$	$\mathbf{w}_2 = [2436.97, -810.07]$
$\beta_3 = 5$	$\mathbf{w}_3 = [0, 0]$

Table 2
The different smoothness levels from abrupt transitions to smooth transitions for the situations shown in Fig. 3(a).

Smoothness level of transitions	1	2	3	4	5	6	7	8	9	10
$ \lambda_k $	$\frac{ \mathbf{w}_{k1} }{1}$	$\frac{ \mathbf{w}_{k1} }{2}$	$\frac{ \mathbf{w}_{k1} }{5}$	$\frac{ \mathbf{w}_{k1} }{10}$	$\frac{ \mathbf{w}_{k1} }{20}$	$\frac{ \mathbf{w}_{k1} }{40}$	$\frac{ \mathbf{w}_{k1} }{50}$	$\frac{ \mathbf{w}_{k1} }{80}$	$\frac{ \mathbf{w}_{k1} }{100}$	$\frac{ \mathbf{w}_{k1} }{125}$

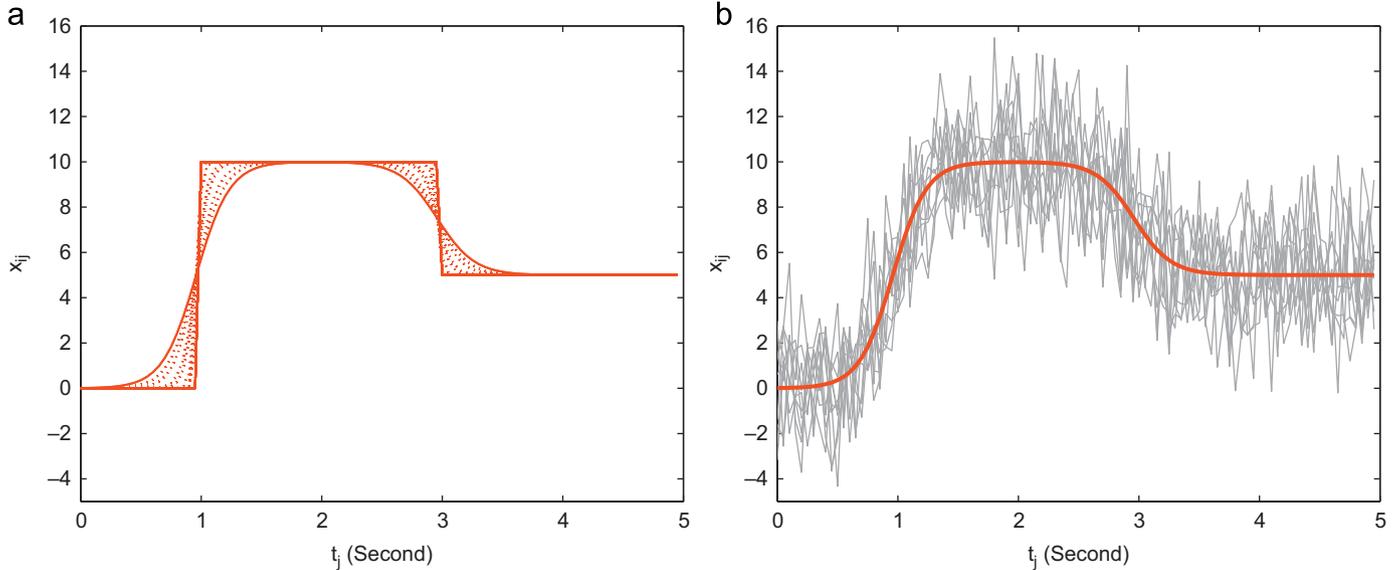


Fig. 3. The true denoised curves from abrupt transitions to smooth transitions for the first experiment (a) and an example of simulated curves ($n = 10, m = 100$) with a smoothness level of transition corresponding to the level 8 in Table 2.

Table 3
Simulation parameters for experiment 2 and experiment 3.

$\beta_1 = [23, -36, 18]$	$\mathbf{w}_1 = [92.72, -46.72]$	$\sigma_1 = 1$
$\beta_2 = [-3.9, 11.08, -2.2]$	$\mathbf{w}_2 = [61.16, -15.28]$	$\sigma_2 = 1.25$
$\beta_3 = [-337, 141.5, -14]$	$\mathbf{w}_3 = [0, 0]$	$\sigma_3 = 0.75$

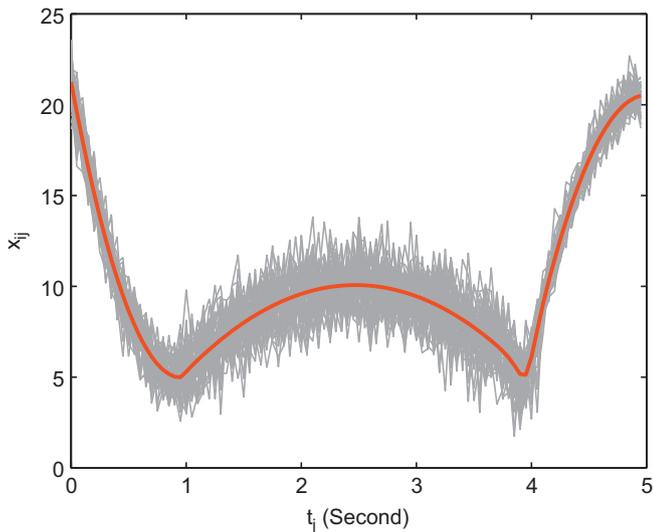


Fig. 4. Example of 50 curves simulated according to the proposed regression model with a curves size $m = 100$, for the second and the third experiment.

For each value of n , each value of m and each value of the smoothness level of transitions, the values of assessment criteria were averaged over 20 different curves samples. Fig. 5 shows the error of curves modeling (approximation error) in relation to the

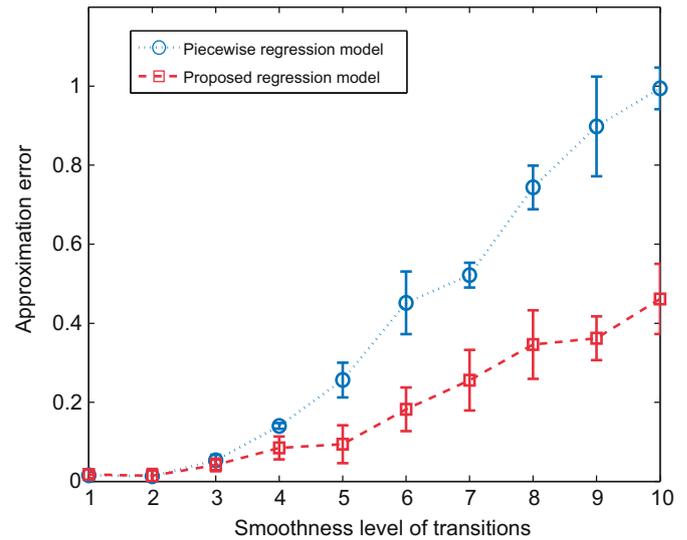


Fig. 5. Approximation error in relation to the smoothness level of transitions, obtained with the proposed approach (square) and the piecewise polynomial regression approach (circle).

smoothness level of transitions. It can be seen that, for abrupt transitions (levels 1, 2 and 3), the two approaches provides similar results. However, when the curves present smooth transitions, the proposed approach provides more accurate results than the piecewise regression approach.

For the second and the third experiments, it can be seen in both Figs. 6 and 7 that the curves modeling error decreases when the curves size m and the number of curves n increase for the two approaches. The results provided by the proposed model are more accurate than those of the piecewise regression approach.

Finally, Fig. 8 shows that the computation time of the proposed algorithm does not increase much, while that of the piecewise approach grows considerably with the number of curves and with the curves size.

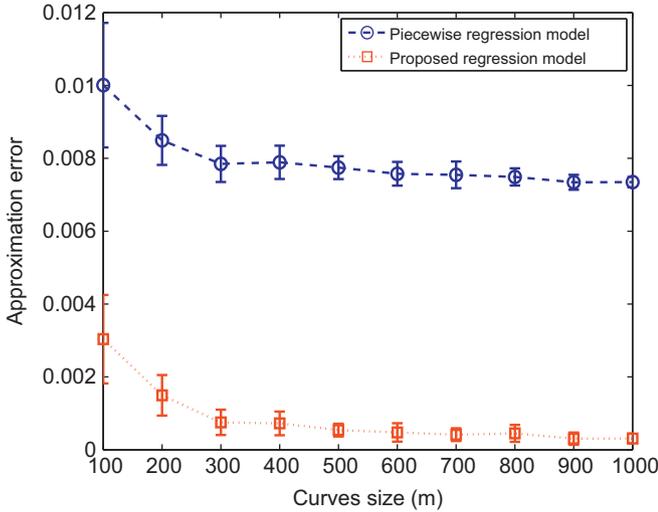


Fig. 6. Approximation error in relation to the curves size m for $n=50$ curves, obtained with the proposed approach (square) and the piecewise polynomial regression approach (circle).

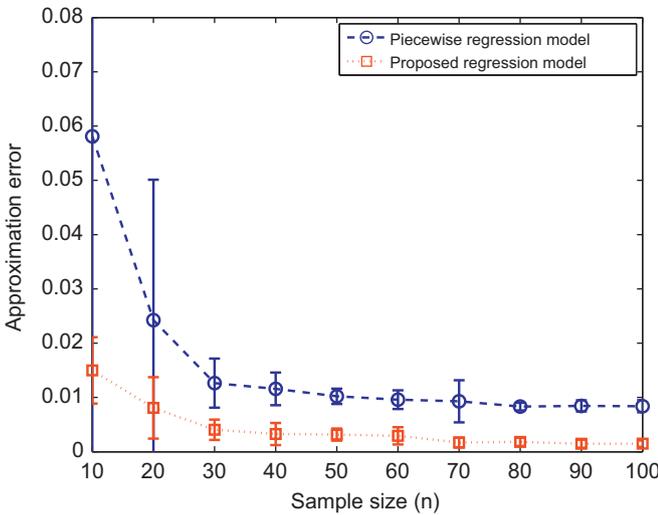


Fig. 7. Approximation error in relation to the number of curves n for a curves size $m=100$, obtained with the proposed approach (square) and the piecewise polynomial regression approach (circle).

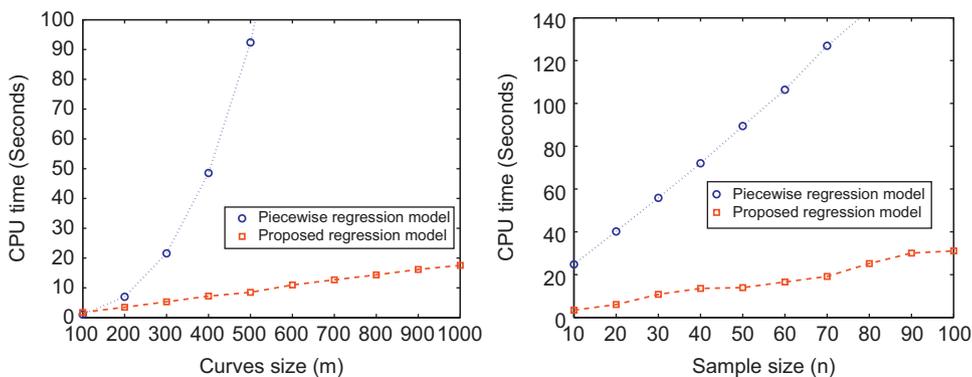


Fig. 8. Average running time (in second) in relation to the curves size m for $n=50$ curves (left) and in relation to the number of curves n for a curves size $m=500$ (right), obtained with the proposed approach (square) and the piecewise polynomial regression approach (circle).

4.2. Evaluation in terms of curve classification

This section is concerned with the evaluation of the proposed approach in terms of curve classification. Two types of data sets are considered: the waveform data set of Breiman and a real-world data set from railway switch operations.

4.2.1. Waveform curves of Breiman

In this part, the proposed approach is evaluated in terms of curve classification by considering the waveform data introduced in [3] and studied in [12,26] and elsewhere. The waveform data consist in a three-class problem where each curve is generated as follows:

- $\mathbf{x}_1(t) = uh_1(t) + (1-u)h_2(t) + \varepsilon_t$ for the class 1;
- $\mathbf{x}_2(t) = uh_2(t) + (1-u)h_3(t) + \varepsilon_t$ for the class 2;
- $\mathbf{x}_3(t) = uh_1(t) + (1-u)h_3(t) + \varepsilon_t$ for the class 3;

where u is a uniform random variable on $(0, 1)$,

- $h_1(t) = \max(6 - |t - 11|, 0)$;
- $h_2(t) = h_1(t - 4)$;
- $h_3(t) = h_1(t + 4)$;

and ε_t is a zero-mean Gaussian noise with unit standard deviation. The temporal interval considered for each curve is $[0;20]$ with a constant period of sampling of 1 s. Five hundred simulated curves were drawn for each class.

Table 4 shows the average classification error rates and the corresponding standard deviations (in parentheses) obtained with the two approaches. It can be observed that the proposed regression approach provides more accurate discrimination results than those of the piecewise polynomial regression approach.

Figs. 9 and 10 show the curves estimated, respectively, by the piecewise polynomial regression approach and the proposed approach for $K=2$ and $p=3$. We can see that the curve estimated by the piecewise regression approach presents discontinuities since it is computed from a hard segmentation of the curves, while, the curves approximation provided with the proposed

Table 4
Classification results for the waveform curves.

Modeling approach	Test error rates (%)
Piecewise regression model	2.4 (0.64)
Proposed regression model	1.67 (0.84)

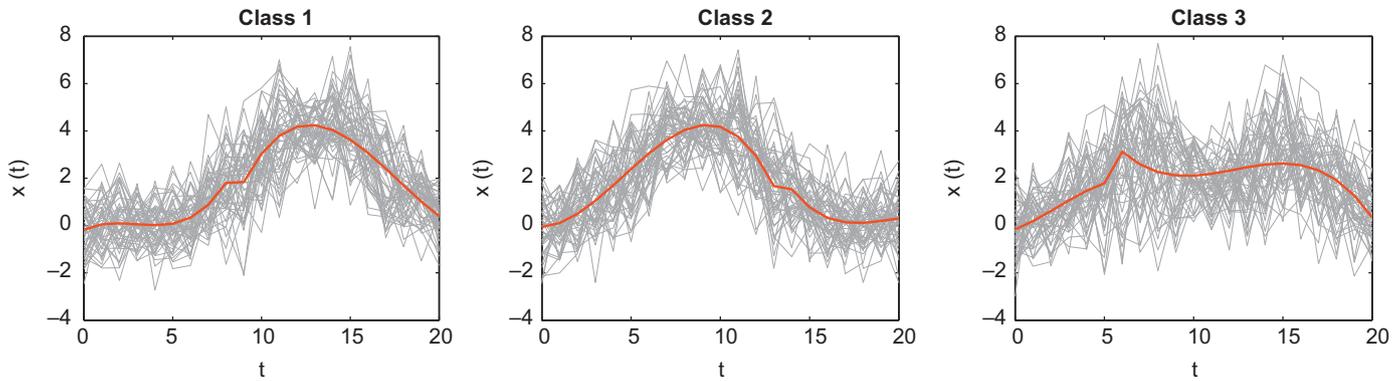


Fig. 9. Some examples of the waveforms for the three classes with 50 curves per class and the estimated model for each class obtained with the piecewise polynomial regression approach.

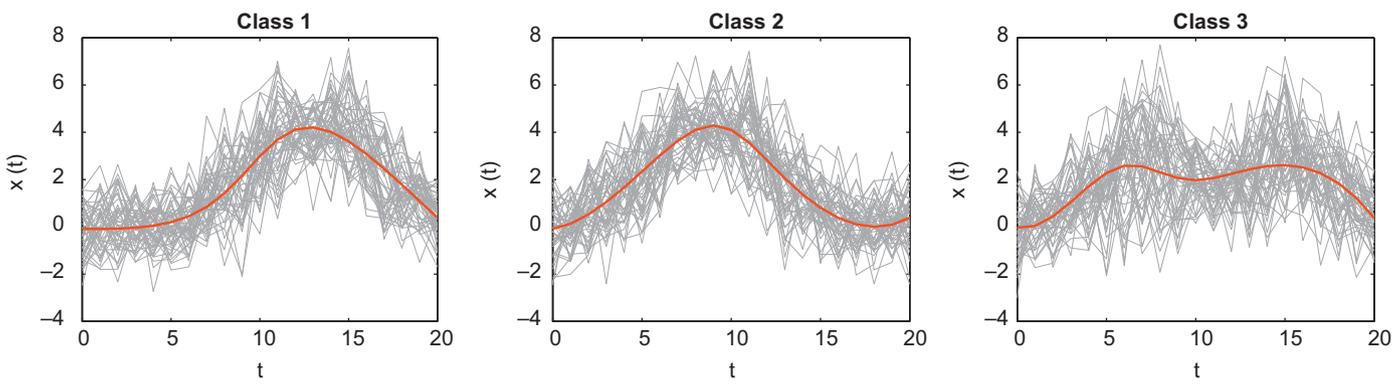


Fig. 10. Some examples of the waveforms for the three classes with 50 curves per class and the estimated model for each class obtained with the proposed approach.

Table 5
Classification results for the switch operation curves.

Modeling approach	Test error rates (%)
Piecewise regression model	1.82 (5.74)
Proposed regression model	1.67 (2.28)

regression model is continuous due to the use of the logistic function adapted to both smooth and abrupt regime changes.

4.2.2. Real-world curves

This section is devoted to an evaluation of the proposed approach in terms of curve classification using real curves from switch operations. A database of 120 curves subdivided into three classes was used:

- $g=1$: no defect class;
- $g=2$: minor defect class;
- $g=3$: critical defect class.

The cardinal numbers of the three classes are $n_1=35$, $n_2=40$ and $n_3=45$, respectively. The results in terms of misclassification error rates are given in Table 5.

We can see that the proposed approach provides results slightly better than those of the piecewise regression approach. Although the difference in terms of misclassification error is not very significant, the proposed method ensures, unlike the piece-

wise regression approach, the continuity of the estimated curves (see Figs. 11 and 12). Since the transitions involved in the segments 1 and 5 are abrupt, they are well estimated by the two approaches. However, the segments 2 and 4 estimated by the proposed approach have been found more realistic regarding the true phases involved in a real switch operation.

It should be mentioned that, despite the very good results obtained for curves description, this approach may have limitations in terms of curve classification. The next section illustrates this limitation through simulations.

4.3. Behavior of the proposed approach for complex shaped classes

The aim of this part is to show the behavior of the proposed classification approach for classes having complex non-convex shapes. We consider simulated curves from two classes:

- Class 1: This class consists of 40 curves simulated with the generative model presented in Section 3.3. Fifteen curves are simulated with the parameters estimated from the first class of the real dataset (see Fig. 12 (left)) and 25 curves are simulated with the parameters estimated from the second class (see Fig. 12 (middle)).
- Class 2: This class consists of 37 curves simulated in the following manner: 17 curves are simulated with the parameters estimated from the second class of the real data and 20 curves are simulated with the parameters estimated from the third class (cf. Fig. 12 (middle) and Fig. 12 (right), respectively).

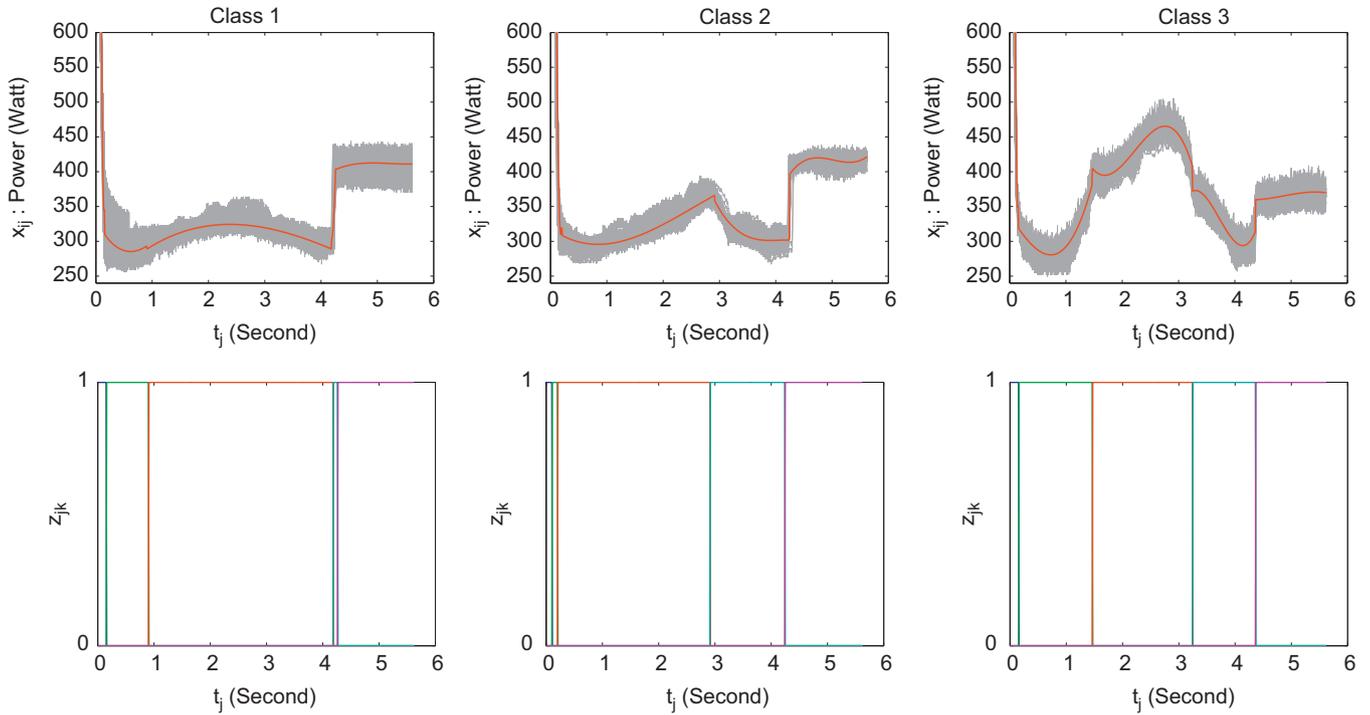


Fig. 11. The three classes of switch operation curves and the corresponding estimated curve (top) and the segmentation (bottom) obtained with the piecewise polynomial regression model.

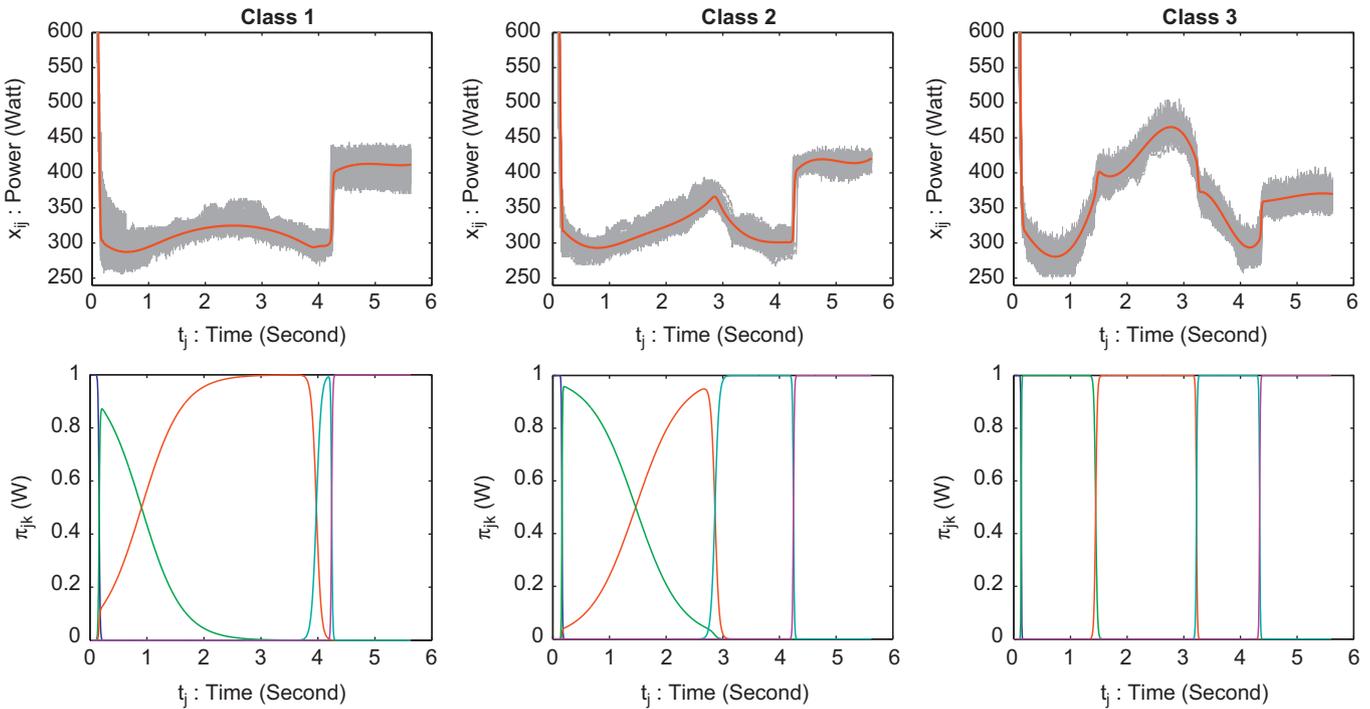


Fig. 12. The three classes of the switch operation curves and the estimated curves and the corresponding estimated logistic probabilities for each class of curves obtained provided by the proposed approach.

Fig. 13 shows the simulated curves, the estimated curves approximation and the estimated logistic probabilities.

In this setting, the classification error rate obtained with the proposed approach is 20% with a standard deviation of 8.16%. The poor performances in this case can be attributed to the non-homogeneous nature of the simulated groups. As it can be observed in Fig. 13, especially for class 2, the proposed model is not adapted for classes having complex shape.

5. Conclusion

This paper introduces a new approach for functional data description. The proposed approach consists in a regression model governed by a discrete hidden process. The logistic functions used as the probability distributions of the hidden variables allow for smooth or abrupt transitions between various polynomial regression components over time. A curves discrimination

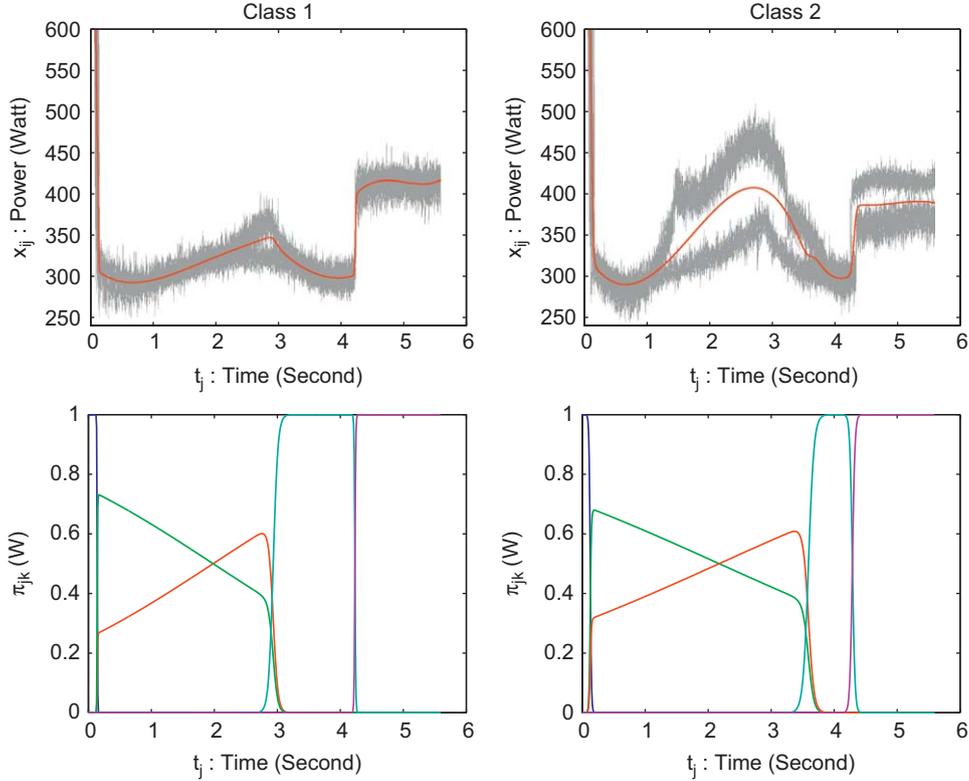


Fig. 13. Two complex classes (40 curves from class 1 and 37 curves from class 2) generated according to the generative model presented in Section 3.3.

method is derived by applying the Maximum A Posteriori rule. An experimental study performed on simulated data and real curves acquired during switch operations reveals good performances of the proposed approach in terms of curve modeling and classification, compared to the piecewise polynomial regression approach. The limitations of the proposed approach in terms of classification have been shown for complex shaped classes. A future work will consist in considering a more efficient approach to deal with these limitations, where a complex shaped class will be modeled by a mixture of hidden process regression models.

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Appendix A. The EM algorithm

In the context of maximizing the likelihood by the EM algorithm, the complete log-likelihood [7] is written as

$$\begin{aligned}
 CL(\theta; \mathcal{X}, \mathbf{z}) &= \log p(\mathbf{x}_1, \dots, \mathbf{x}_n, \mathbf{z} | \mathbf{x}; \theta) \\
 &= \log \prod_{i=1}^n \prod_{j=1}^m \prod_{k=1}^K [p(z_j = k; \mathbf{w}) p(x_{ij} | z_j = k; \theta)]^{z_{jk}} \\
 &= \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^K z_{jk} \log [\pi_{jk}(\mathbf{w}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2)]. \quad (28)
 \end{aligned}$$

The EM algorithm starts from an initial parameter $\theta^{(0)}$ and alternates the two following steps until convergence:

E step (expectation): This step computes the conditional expectation of the complete log-likelihood given the observations and the current value $\theta^{(q)}$:

$$\begin{aligned}
 Q(\theta, \theta^{(q)}) &= E[CL(\theta; \mathcal{X}, \mathbf{z}) | \mathcal{X}; \theta^{(q)}] \\
 &= \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^K E(z_{jk} | x_{ij}; \theta^{(q)}) \log [\pi_{jk}(\mathbf{w}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2)] \\
 &= \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^K \tau_{ijk}^{(q)} \log [\pi_{jk}(\mathbf{w}) \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2)] \\
 &= \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^K \tau_{ijk}^{(q)} \log \pi_{jk}(\mathbf{w}) \\
 &\quad + \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^K \tau_{ijk}^{(q)} \log \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2),
 \end{aligned}$$

where $\tau_{ijk}^{(q)}$ is the posterior probability that x_{ij} originates from the k th regression model defined by Eq. (20).

As shown in the expression of Q , this step simply requires the computation of $\tau_{ijk}^{(q)}$.

M step (maximization): This step updates the value of the parameter θ by maximizing Q with respect to θ . To perform this maximization, we can see that Q is written as

$$Q(\theta, \theta^{(q)}) = Q_1(\mathbf{w}) + \sum_{k=1}^K Q_2(\beta_k, \sigma_k^2), \quad (29)$$

with

$$Q_1(\mathbf{w}) = \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^K \tau_{ijk}^{(q)} \log \pi_{jk}(\mathbf{w}) \quad (30)$$

and

$$Q_2(\beta_k, \sigma_k^2) = \sum_{i=1}^n \sum_{j=1}^m \tau_{ijk}^{(q)} \log \mathcal{N}(x_{ij}; \beta_k^T \mathbf{r}_j, \sigma_k^2)$$

$$= -\frac{1}{2} \left[\frac{1}{\sigma_k^2} \sum_{i=1}^n \sum_{j=1}^m \tau_{ijk}^{(q)} (x_{ij} - \beta_k^T \mathbf{r}_j)^2 + nm_k^{(q)} \log \sigma_k^2 \right] - \frac{nm_k^{(q)}}{2} \log 2\pi; \quad k = 1, \dots, K, \quad (31)$$

where $m_k^{(q)} = \sum_{j=1}^m \tau_{ijk}^{(q)}$ can be seen as the number of elements in component k estimated at iteration q for each curve \mathbf{x}_i . Thus, the maximization of Q can be performed by separately maximizing $Q_1(\mathbf{w})$ with respect to \mathbf{w} and $Q_2(\beta_k, \sigma_k^2)$ with respect to (β_k, σ_k^2) for $k = 1, \dots, K$.

Maximizing Q_2 with respect to β_k consists in analytically solving a weighted least-squares problem. The estimates are given by

$$\beta_k^{(q+1)} = \arg \min_{\beta_k} \sum_{i=1}^n \sum_{j=1}^m \tau_{ijk}^{(q)} (x_{ij} - \beta_k^T \mathbf{r}_j)^2 = (A^T W_k^{(q)} A)^{-1} A^T W_k^{(q)} \mathcal{X}. \quad (32)$$

Maximizing Q_2 with respect to σ_k^2 provides the following updating formula:

$$\sigma_k^{2(q+1)} = \arg \min_{\sigma_k^2} \left[\frac{1}{\sigma_k^2} \sum_{i=1}^n \sum_{j=1}^m \tau_{ijk}^{(q)} (x_{ij} - \beta_k^{T(q+1)} \mathbf{r}_j)^2 + nm_k^{(q)} \log \sigma_k^2 \right] = \frac{1}{nm_k^{(q)}} \sum_{i=1}^n \sum_{j=1}^m \tau_{ijk}^{(q)} (x_{ij} - \beta_k^{T(q+1)} \mathbf{r}_j)^2. \quad (33)$$

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