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Cluster weighted models for functional data*

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Abstract

We propose a method, funWeightClust, based on a family of parsimonious models for clustering heterogeneous functional linear regression data. These models extend cluster weighted models to functional data, and they allow for multivariate functional responses and predictors. The proposed methodology follows the approach used by the functional high dimensional data clustering (funHDDC) method. We construct an expectation maximization (EM) algorithm for parameter estimation. Using simulated and benchmark data we show that funWeightClust outperforms funHDDC and several two-steps clustering methods. We also use funWeightClust to analyze traffic patterns in Edmonton, Canada.

Keywords: Model based clustering, Cluster weighted models, Functional linear regression, EM algorithm, Multivariate functional responses, Multivariate functional principal component analysis

1 Introduction

The rapid and extensive development of data-intensive technologies has lead to an increased demand for efficient methods to analyze complex data. Internet of Things (IoT) embedded devices, such as cars, smart watches, and thermostats, record a lot of functional data for which the observations are represented by functions ([Ramsay and Silverman, 2006](#)). Examples of functional data are the average daily temperature over a period of time, the daily stock trading prices in financial markets, and the signal recorded in an electrocardiogram (ECG). For complex applications many times it is

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necessary to start by using unsupervised learning algorithms to identify homogeneous groups of data, i.e. clustering the data. Here we propose a new model based clustering method, funWeightClust, for data that have a functional linear regression relationship between the variables.

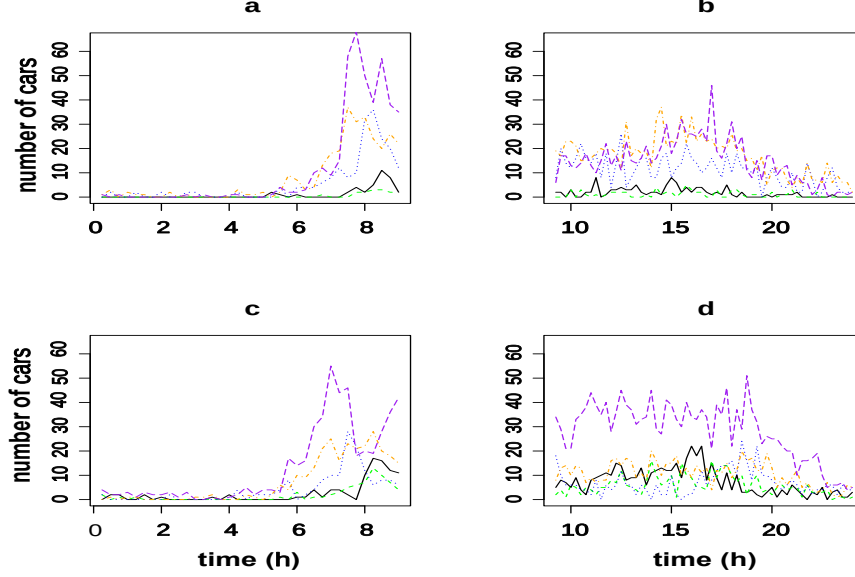


Fig. 1 Edmonton traffic data: cars going 5-10 km/h under the speed limit a) from 12 a.m. to 8 a.m. b) from 8:15 a.m. to 11:45 p.m.; cars going 0-5 km/h over the speed limit c) from 12 a.m. to 8 a.m. d) from 8:15 a.m. to 11:45 p.m.. Roads with a maximum speed of 30 km/h (black plain lines), 40 km/h (green dashed lines), 50 km/h (blue dotted lines), 60 km/h (orange dot-dashed lines) and 70 km/h (purple dashed lines).

This work was motivated by the study of traffic flow in Edmonton, Canada. The city of Edmonton collects a large amount of data about traffic flow that characterizes road activity. In Figure 1 a,b we plot a few curves corresponding to car counts going 5-10 km/h under the speed limit, and in Figure 1 c, d we plot curves for car counts going 0-5 km/h over the speed limit. The data is recorded every 15 minutes and we use different colors and line types to distinguish between the curves corresponding to data collected on roads with various maximum speed limits. The morning traffic rush from 12 a.m. to 8 a.m. is included in Figure 1 a, c and the afternoon traffic from 8:15 a.m. to 11:45 p.m. in Figure 1 b, d. An initial step of traffic analysis is to partition the data in homogeneous groups. The afternoon traffic flow depends on the morning traffic flow, and functional linear regression can model this relationship. Given the nature of the traffic data we have to consider a model that allows for multivariate functional response and predictors, and, to the best of our knowledge, none of the existing clustering methods (Yao et al, 2011, Conde et al, 2021, Wang et al, 2016, Chamroukhi, 2016) deals with multivariate functional responses.

Time series are also functional data, and special models are used for time series analysis (e.g. the recent work in [Dama and Sinoquet, 2023](#)), but here we focus on functional linear regression models. Our approach extends multivariate cluster weighted models ([Dang et al, 2017](#)) to functional data, based on the framework used by the funHDDC method ([Bouveyron and Jacques, 2011](#), [Schmutz et al, 2020](#)). We assume that the data are collected on an one-dimensional interval and with a regular sampling scheme from the pairs $(\mathbf{Y}_1, \mathbf{X}_1), \dots, (\mathbf{Y}_n, \mathbf{X}_n)$ of multivariate curves. For example, for the Edmonton traffic data the bi-dimensional covariate or predictors curves $\mathbf{X}_i$ correspond to the morning rush and are plotted in Figure 1 a,c, and the bi-dimensional response curves $\mathbf{Y}_i$ correspond to the afternoon traffic illustrated in Figure 1 b,d. We want to cluster the observations in homogeneous groups and we assume that clusterwise the data come from a functional linear regression model.

One of the difficulties when clustering functional data is that these data live in an infinite dimensional space and the notion of probability density function generally does not exist ([Delaigle and Hall, 2010](#)). Thus model-based methods are not directly available for functional data, so we follow the same approach used for the funHDDC method ([Bouveyron and Jacques \(2011\)](#), [Jacques and Preda \(2013\)](#), [Schmutz et al \(2020\)](#)). We first decompose the functional data in a basis of functions (such as Fourier series, B-splines, etc.), then we construct a probabilistic model for the basis coefficients.

The main contributions of this paper are:

- We propose a model based clustering method, funWeightClust, based on functional linear regression models with multivariate functional response and predictors.
- funWeightClust extends the approach used for the funHDDC ([Bouveyron and Jacques, 2011](#), [Schmutz et al, 2020](#)) to clustering functional data that include covariates. We use multivariate functional principal component analysis (MFPCA) ([Jacques and Preda, 2014b](#)) and we assume that the scores have multivariate normal distributions.
- We add flexibility to the model by including also the distributions for the covariates, so the proposed approach is also an extension of the cluster weighted models used for multivariate data ([Dang et al, 2017](#)).
- We propose a variant of the Expectation-Maximization (EM) algorithm that allows to learn the parameters of our model.
- We consider several parsimonious models.

The paper is organized as follows. Related work is reviewed in Section 2. The cluster weighted models for functional data are constructed in Section 3. In Section 4 a learning algorithm to estimate the model parameters is derived and computational details are presented. Next, Section 5 includes experimental results for both simulated and real-world data and a discussion of the performance of the proposed approach. Finally, in Section 6 we provide concluding remarks and future directions.

2 Related work

Clustering techniques that account for regression relationships between multivariate data can be also applied to functional data if we use one of the following two approaches

(Jacques and Preda, 2014a). The first approach is a raw-data clustering, and it consists of directly applying multivariate clustering techniques to the finite discretizations of the functions. The second approach is to use a two-step method and first do a decomposition of the functional data in a basis of functions (such as Fourier series, B-splines, etc.), and then directly apply multivariate clustering methods to the basis coefficients. Next, we will summarize some of the model based clustering methods for multivariate data with linear regression relationships between the variables.

Finite mixture of regression (FMR) (DeSarbo and Cron, 1988) are mixture based methodologies that deal with clusterwise linear regression. They are implemented in the *flexmix* R package (Leisch, 2004) and the implementation allows multivariate uncorrelated responses. However, as in the classical regression analysis, the model assumes that the covariates are fixed and the assignment of the data to clusters is not dependent on the distribution of the covariates.

Cluster weighted models (CWM) were first introduced in Gershensfeld (1997) and they take into account the distribution of the covariates. In the simplest form it is assumed that both the response and the covariates have normal distributions. Some extensions of this methodology considers t-distributions (Ingrassia et al, 2012), contaminated normal distributions (Punzo and McNicholas, 2017), and various types of response variables and covariates of mixed-type (Ingrassia et al, 2015, Punzo and Ingrassia, 2016). The R package *flexCWM* (Mazza et al, 2018) implements models for which the conditioned response variable has some of the most common distributions of the exponential family or the t-distribution. However, these CWMs consider univariate responses, so they cannot be applied to finite discretization of functions or the coefficients corresponding to the decomposition of the functional data in a basis of functions. Very few CWMs consider multivariate responses (Punzo and McNicholas, 2017, Dang et al, 2017).

In (Dang et al, 2017) a CWM with multivariate correlated responses is constructed. We assume that the response vector $\mathbf{Y} : \Omega \rightarrow \mathbb{R}^d$, the vector of covariates $\mathbf{X} : \Omega \rightarrow \mathbb{R}^p$, Ω is partitioned into G distinct groups, $\Omega = \Omega_1 \cup \dots \cup \Omega_G$, and

$$\mathbf{X}|\Omega_g \sim N(\boldsymbol{\mu}_X, \boldsymbol{\Sigma}_X), \quad \mathbf{Y}|\mathbf{X} = \mathbf{x}, \Omega_g \sim N(\mathbf{B}_g^\top \mathbf{x}^*, \boldsymbol{\Sigma}_Y), \quad \mathbf{x}^* = (1, \mathbf{x}^\top)^\top,$$

where $\mathbf{B}_g$ is the $(p+1) \times d$ matrix of regression coefficients. The joint probability $p(\mathbf{x}, \mathbf{y})$ of $\mathbf{X}, \mathbf{Y}$ can be written as

$$p(\mathbf{x}, \mathbf{y}) = \sum_{g=1}^G \pi_g \phi(\mathbf{y}; \mathbf{B}_g^\top \mathbf{x}^*, \boldsymbol{\Sigma}_Y) \phi(\mathbf{x}; \boldsymbol{\mu}_X, \boldsymbol{\Sigma}_X), \quad (1)$$

where ϕ represent the density of the Gaussian distribution, and $\pi_g > 0$ are the mixing weights with $\sum_{g=1}^G \pi_g = 1$. Here we consider this type of model clusterwise for the coefficients of functional data.

Recently finite mixtures of matrix-variate regressions have been considered by Melnykov and Zhu (2019) and matrix-variate CWMs are constructed in Tomarchio et al (2021). Moreover, the multivariate response CWM (1) was extended for the family of models with skewed distributions in Gallagher et al (2022).

In addition to these methods for clustering multivariate data, there is a vast literature in functional linear regression (FLR) (Ramsay and Silverman, 2006, Ferraty and Vieu, 2006, Horváth and Kokoszka, 2012). A large variety of FLR models was proposed, but the majority of them consider a scalar response, or a single functional response, and one or more functional predictors. A multivariate FLR model (mFLR) with both multivariate functional response and predictor is constructed in Chiou et al (2016):

$$Y_k(t) = \sum_{l=1}^p \int_{\mathcal{T}} \beta_{0lk}(s, t) X_l(s) ds + \xi_k(t), \quad k = 1, \dots, d, \quad (2)$$

where $\{X_l\}_{1 \leq l \leq p}$ and $\{Y_k\}_{1 \leq k \leq d}$ are the predictor and response variables, respectively, $\mathcal{T}$ is a closed interval, $\beta_{0lk}(s, t)$ is the bivariate regression coefficient function, and $\xi_k(t)$ is the random error process. Estimations, predictions, and asymptotic properties of this mFLR model are also discussed in Chiou et al (2016). We extend these mFLR models to multivariate functional mixtures models that could be used in applications where observations might come from an inhomogeneous population with several homogeneous clusters. We assume that for each cluster c we have a model like (2), but with cluster specific regression coefficients $\beta_{0lk}^{(c)}(s, t)$.

To the best of our knowledge there are not many papers that consider mixtures of functional linear regression models for clustering. In Chiou (2012) conditional of cluster membership, a model similar with (2), but with single functional response and predictor ($p = d = 1$) and different regression coefficients $\beta^{(c)}(s, t)$ for each cluster c , is used for classification and prediction of traffic data. The classification method is based on subspace projection.

In Yao et al (2011) a functional regression model is used for clustering. In each cluster the model is a simpler version of (2), where the response is a scalar $Y(t) = Y \in \mathbb{R}$, there is only one functional predictor ($p = 1$) and the univariate regression coefficient function $\beta^{(c)}(s)$ has specific values for each cluster c . The idea of the clustering method is to use functional principal components analysis to reduce the functional model to a classical mixture of linear regressions models.

In Conde et al (2021) a cluster-specific model similar with (2), with a single functional response and multiple functional predictors ($d = 1, p \geq 1$), and different regression coefficients $\beta_{0l}^{(c)}(s, t)$, $l = 1, \dots, p$ for each cluster c , is used for finding clusters in a gene expression time course data set. The model is fitted using boosting.

A mixture constructed with a different type of models, called concurrent functional linear models, is used in Wang et al (2016) to analyze the CO₂ emissions - GDP relationship. For each cluster c

$$Y(t) = \sum_{l=1}^p \beta_l^{(c)}(t) X_l(t) + \xi^{(c)}(t), \quad (3)$$

where $\{X_l\}_{1 \leq l \leq p}$ and Y are the predictor and response variables, $\beta_l^{(c)}(t)$ is the cluster specific regression coefficient function, and $\xi^{(c)}(t)$ is the random error process. The estimation is done combining the EM algorithm with kernel regression and functional principal components analysis. In Chamroukhi (2016) polynomial, spline, and B-spline

regression mixtures with a single functional response and multiple functional predictors are used for clustering data. The model is fitted considering a penalized maximum likelihood and an EM like algorithm.

3 Multivariate functional cluster weighted model

For any compact interval $\mathcal{T}$ in $\mathbb{R}$, we consider the Hilbert space $L^2(\mathcal{T}) = \{f : \mathcal{T} \rightarrow \mathbb{R}, \int_{\mathcal{T}} f^2(t)dt < \infty\}$ with the inner product $\langle f, g \rangle = \int_{\mathcal{T}} f(t)g(t)dt$ and the norm $\|f\| = \langle f, f \rangle^{1/2}$ (Ramsay and Silverman, 2006).

We assume that the n p_Y -variate response curves $\{\mathbf{Y}_1, \dots, \mathbf{Y}_n\}$ are independent realizations of a L^2 - continuous stochastic process $\mathbf{Y} = \{\mathbf{Y}(t)\}_{t \in \mathcal{T}_Y} = \{(Y^1(t), \dots, Y^{p_Y}(t))^\top\}_{t \in \mathcal{T}_Y} \in \mathbb{H}_Y$, where $\mathcal{T}_Y \subset \mathbb{R}$ is a compact interval and $\mathbb{H}_Y := \{\mathbf{f} = (f_1, \dots, f_{p_Y})^\top : \mathcal{T}_Y \rightarrow \mathbb{R}^{p_Y}, f_i \in L^2(\mathcal{T}_Y), i = 1, \dots, p_Y\}$ is a Hilbert space with the inner product $\langle \mathbf{f}, \mathbf{g} \rangle_{\mathbb{H}_Y} = \sum_{l=1}^{p_Y} \langle f_l, g_l \rangle$ and the norm $\|\mathbf{f}\|_{\mathbb{H}_Y} = \langle \mathbf{f}, \mathbf{f} \rangle_{\mathbb{H}_Y}^{1/2}$.

Similarly we assume that the n p_X -variate covariate curves $\{\mathbf{X}_1, \dots, \mathbf{X}_n\}$ are independent realizations of a L^2 - continuous stochastic process $\mathbf{X} = \{\mathbf{X}(t)\}_{t \in \mathcal{T}_X} = \{(X^1(t), \dots, X^{p_X}(t))^\top\}_{t \in \mathcal{T}_X} \in \mathbb{H}_X$, where $\mathcal{T}_X \subset \mathbb{R}$ is a compact interval and $\mathbb{H}_X := \{\mathbf{f} = (f_1, \dots, f_{p_X})^\top : \mathcal{T}_X \rightarrow \mathbb{R}^{p_X}, f_i \in L^2(\mathcal{T}_X), i = 1, \dots, p_X\}$ is a Hilbert space with the inner product $\langle \mathbf{f}, \mathbf{g} \rangle_{\mathbb{H}_X} = \sum_{j=1}^{p_X} \langle f_j, g_j \rangle$ and the norm $\|\mathbf{f}\|_{\mathbb{H}_X} = \langle \mathbf{f}, \mathbf{f} \rangle_{\mathbb{H}_X}^{1/2}$.

For each pair of curves $(\mathbf{Y}_i, \mathbf{X}_i)$ we have access to a finite set of values $y_i^{s_Y}(t_{i1}^Y) \dots, y_i^{s_Y}(t_{im_i}^Y), x_i^{s_X}(t_{i1}^X) \dots, x_i^{s_X}(t_{in_i}^X)$, where $t_{i1}^Y < t_{i2}^Y < \dots < t_{im_i}^Y, t_{i1}^X < t_{i2}^X < \dots < t_{in_i}^X, t_{ij}^Y \in \mathcal{T}_Y, t_{il}^X \in \mathcal{T}_X, j = 1, \dots, m_i, l = 1, \dots, n_i, s_Y = 1, \dots, p_Y, s_X = 1, \dots, p_X, i = 1, \dots, n$. To reconstruct the functional form of the data we assume that the curves belong to a finite dimensional space, and we have:

$$Y_i^l(t) = \sum_{r=1}^{R_l^Y} c_{Y,ir}^l \xi_{Y,r}^l(t), \quad X_i^j(t) = \sum_{r=1}^{R_j^X} c_{X,ir}^j \xi_{X,r}^j(t). \quad (4)$$

Here $\{\xi_{Y,r}^l\}_{1 \leq r \leq R_l^Y}$ is the basis for the l^{th} components of the multivariate curves $\{\mathbf{Y}_1, \dots, \mathbf{Y}_n\}$, $c_{Y,ir}^l$ are the coefficients, and R_l^Y is the number of basis functions. Similarly for the covariate curves $\{\mathbf{X}_1, \dots, \mathbf{X}_n\}$, $\{\xi_{X,r}^j\}_{1 \leq r \leq R_j^X}$ is the basis for the j^{th} components, $c_{X,ir}^j$ are the coefficients, and R_j^X is the number of basis functions.

Gathering the coefficients and the basis functions we rewrite (4) as

$$\mathbf{Y}(t) = \mathbf{C}_Y \boldsymbol{\xi}_Y^\top(t), \quad \mathbf{Y}(t) = (\mathbf{Y}_1(t), \dots, \mathbf{Y}_n(t))^\top, \quad (5)$$

$$\mathbf{X}(t) = \mathbf{C}_X \boldsymbol{\xi}_X^\top(t), \quad \mathbf{X}(t) = (\mathbf{X}_1(t), \dots, \mathbf{X}_n(t))^\top, \quad (6)$$

with

$$\begin{aligned}
\mathbf{C}_Y &= \begin{pmatrix} c_{Y,11}^1 & \cdots & c_{Y,1R_1^Y}^1 & c_{Y,11}^2 & \cdots & c_{Y,1R_2^Y}^2 & \cdots & c_{Y,11}^{p_Y} & \cdots & c_{Y,1R_{p_Y}^Y}^{p_Y} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ c_{Y,n1}^1 & \cdots & c_{Y,nR_1^Y}^1 & c_{Y,n1}^2 & \cdots & c_{Y,nR_2^Y}^2 & \cdots & c_{Y,n1}^{p_Y} & \cdots & c_{Y,nR_{p_Y}^Y}^{p_Y} \end{pmatrix}, \\
\boldsymbol{\xi}_Y(t) &= \begin{pmatrix} \xi_{Y,1}^1(t) & \cdots & \xi_{Y,R_1^Y}^1 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \xi_{Y,1}^2(t) & \cdots & \xi_{Y,R_2^Y}^2(t) & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \cdots & \xi_{Y,1}^{p_Y}(t) & \cdots & \xi_{Y,R_{p_Y}^Y}^{p_Y}(t) \end{pmatrix}, \\
\mathbf{C}_X &= \begin{pmatrix} c_{X,11}^1 & \cdots & c_{X,1R_1^X}^1 & c_{X,11}^2 & \cdots & c_{X,1R_2^X}^2 & \cdots & c_{X,11}^p & \cdots & c_{X,1R_p^X}^p \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ c_{X,n1}^1 & \cdots & c_{X,nR_1^X}^1 & c_{X,n1}^2 & \cdots & c_{X,nR_2^X}^2 & \cdots & c_{X,n1}^p & \cdots & c_{X,nR_p^X}^p \end{pmatrix}, \\
\boldsymbol{\xi}_X(t) &= \begin{pmatrix} \xi_{X,1}^1(t) & \cdots & \xi_{X,R_1^X}^1 & 0 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \xi_{X,1}^2(t) & \cdots & \xi_{X,R_2^X}^2(t) & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 & \cdots & \xi_{X,1}^{p_X}(t) & \cdots & \xi_{X,R_{p_X}^X}^{p_X}(t) \end{pmatrix}.
\end{aligned}$$

We want to cluster the n observed response and covariate curves $\{(\mathbf{y}_1, \mathbf{x}_1), \dots, (\mathbf{y}_n, \mathbf{x}_n)\}$ in K homogeneous groups. We suppose that there exists a latent variable $\mathbf{Z}_i = (Z_{i1}, \dots, Z_{iK})^\top$, associated to each observation $(\mathbf{y}_i, \mathbf{x}_i)$, where $Z_{ik} = 1$ if the observation $(\mathbf{y}_i, \mathbf{x}_i)$ belongs to the cluster k and $Z_{ik} = 0$ otherwise. We assume that for every $k \in \{1, \dots, K\}$, given that $Z_{ik} = 1$, the observations come from the following model:

$$\mathbf{Y}_i(t) = \beta_0^k(t) + \int_{\mathcal{T}_X} \beta^k(t, s) \mathbf{X}_i(s) ds + \mathbf{E}^k(t), \quad t \in \mathcal{T}_Y, \quad i = 1, \dots, n. \quad (7)$$

Here $\mathbf{E}^k(t) = (E_1^k(t), \dots, E_{p_Y}^k(t))^T$ is the random error process which is uncorrelated with $\mathbf{X}_i(s)$ for any $(s, t) \in \mathcal{T}_X \times \mathcal{T}_Y$, and for which we have the expansions

$$E_l^k(t) = \sum_{r=1}^{R_l^Y} \epsilon_{0,l}^{k,r} \xi_{Y,r}^l(t), \quad l = 1, \dots, p_Y. \quad (8)$$

Let $R^X := \sum_{j=1}^{p_X} R_j^X$ and $R^Y := \sum_{l=1}^{p_Y} R_l^Y$. We assume that $\boldsymbol{\epsilon}_0^k \sim N(\mathbf{0}, \boldsymbol{\Sigma}_{Y,k})$, where $\boldsymbol{\epsilon}_0^k = (\epsilon_{0,1}^{k,1}, \dots, \epsilon_{0,1}^{k,R_1^Y}, \dots, \epsilon_{0,p_Y}^{k,1}, \dots, \epsilon_{0,p_Y}^{k,R_{p_Y}^Y})^\top \in \mathbb{R}^{R^Y}$.

For the regression coefficients $\beta_0^k(t) = (\beta_{0,1}^k(t), \dots, \beta_{0,p_Y}^k(t))^T$ and the $p_Y \times p_X$ matrix $\boldsymbol{\beta}^k(t, s) = \left(\beta_{lj}^k(t, s) \right)_{\substack{l=1, \dots, p_Y \\ j=1, \dots, p_X}}$ we consider the expansions [\(Ramsay and](#)

Silverman, 2006, Chapter 11.3):

$$\beta_{0,l}^k(t) = \sum_{r=1}^{R_l^Y} \Gamma_{0,l}^{k,r} \xi_{Y,r}^l(t), \quad l = 1, \dots, p_Y \quad (9)$$

$$\beta_{lj}^k(t, s) = \sum_{r_1=1}^{R_l^Y} \sum_{r_2=1}^{R_j^X} \Gamma_{lj}^{k,r_1 r_2} \xi_{Y,r_1}^l(t) \xi_{X,r_2}^j(s), \quad l = 1, \dots, p_Y, \quad j = 1, \dots, p_X. \quad (10)$$

Notice that we have

$$\beta^k(t, s) = \boldsymbol{\xi}_Y(t) \boldsymbol{\Gamma}^k \boldsymbol{\xi}_X(s)^\top, \quad \beta_0^k(t) = \boldsymbol{\xi}_Y(t) \boldsymbol{\Gamma}_0^k, \quad (11)$$

where $\boldsymbol{\Gamma}_0^k = (\Gamma_{0,1}^{k,1}, \dots, \Gamma_{0,1}^{k,R_1^Y}, \dots, \Gamma_{0,p_Y}^{k,1}, \dots, \Gamma_{0,p_Y}^{k,R_{p_Y}^Y})^\top \in \mathbb{R}^{R^Y}$ and

$$\boldsymbol{\Gamma}^k = \begin{pmatrix} \Gamma_{11}^{k,11} & \dots & \Gamma_{11}^{k,1R_1^X} & \Gamma_{12}^{k,11} & \dots & \Gamma_{12}^{k,1R_2^X} & \dots & \Gamma_{1p_X}^{k,11} & \dots & \Gamma_{1p_X}^{k,1R_{p_X}^X} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \dots & \vdots & \ddots & \vdots \\ \Gamma_{11}^{k,R_1^Y 1} & \dots & \Gamma_{11}^{k,R_1^Y R_1^X} & \Gamma_{12}^{k,R_1^Y 1} & \dots & \Gamma_{12}^{k,R_1^Y R_2^X} & \dots & \Gamma_{1p_X}^{k,R_1^Y 1} & \dots & \Gamma_{1p_X}^{k,R_1^Y R_{p_X}^X} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \dots & \vdots & \ddots & \vdots \\ \Gamma_{p_Y 1}^{k,11} & \dots & \Gamma_{p_Y 1}^{k,1R_1^X} & \Gamma_{p_Y 2}^{k,11} & \dots & \Gamma_{p_Y 2}^{k,1R_2^X} & \dots & \Gamma_{p_Y p_X}^{k,11} & \dots & \Gamma_{p_Y p_X}^{k,1R_{p_X}^X} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \dots & \vdots & \ddots & \vdots \\ \Gamma_{p_Y 1}^{k,R_{p_Y}^Y 1} & \dots & \Gamma_{p_Y 1}^{k,R_{p_Y}^Y R_1^X} & \Gamma_{p_Y 2}^{k,R_{p_Y}^Y 1} & \dots & \Gamma_{p_Y 2}^{k,R_{p_Y}^Y R_2^X} & \dots & \Gamma_{p_Y p_X}^{k,R_{p_Y}^Y 1} & \dots & \Gamma_{p_Y p_X}^{k,R_{p_Y}^Y R_{p_X}^X} \end{pmatrix}.$$

Let $\mathbf{W}_X$ be the symmetric block-diagonal $R^X \times R^X$ matrix of inner products between the basis functions:

$$\mathbf{W}_X = \int_{\mathcal{T}_X} \boldsymbol{\xi}_X(s)^\top \boldsymbol{\xi}_X(s) ds,$$

Using (5)-(11), for any $i = 1, \dots, n$ for which $Z_{ik} = 1$ we get ,

$$\begin{aligned} \mathbf{Y}_i^\top(t) &= \mathbf{c}_{Y,i}^\top \boldsymbol{\xi}_Y^\top(t) = \beta_0^k(t)^\top + \int_{\mathcal{T}_X} \mathbf{X}_i^\top(s) \beta^k(t, s)^\top ds + \mathbf{E}^k(t)^\top \\ &= \left(\boldsymbol{\Gamma}_0^k \right)^\top \boldsymbol{\xi}_Y^\top(t) + \mathbf{c}_{X,i}^\top \int_{\mathcal{T}_X} \boldsymbol{\xi}_X^\top(s) \boldsymbol{\xi}_X(s) ds \left(\boldsymbol{\Gamma}^k \right)^\top \boldsymbol{\xi}_Y^\top(t) + (\boldsymbol{\epsilon}_0^k)^\top \boldsymbol{\xi}_Y^\top(t) \\ &= \left(\left(\boldsymbol{\Gamma}_0^k \right)^\top + \mathbf{c}_{X,i}^\top \mathbf{W}_X \left(\boldsymbol{\Gamma}^k \right)^\top + (\boldsymbol{\epsilon}_0^k)^\top \right) \boldsymbol{\xi}_Y^\top(t), \end{aligned}$$

for any $t \in \mathcal{T}_Y$. Here $\mathbf{c}_{X,i}$, $\mathbf{c}_{Y,i}$ are column vectors formed with the coefficients in the i th row of the matrices $\mathbf{C}_X$ and $\mathbf{C}_Y$ respectively. Thus, given that $Z_{ik} = 1$, we obtain

the following model for the column vector formed with the coefficients $\mathbf{c}_{Y,i}$ in the i th row of the matrix $\mathbf{C}_Y$:

$$\mathbf{c}_{Y,i} = \mathbf{\Gamma}_0^k + \mathbf{\Gamma}^k \mathbf{W}_X \mathbf{c}_{X,i} + \boldsymbol{\epsilon}_0^k. \quad (12)$$

If the curves are observed with noise, we use least square smoothing to get the expansion for each curve (Ramsay and Silverman, 2006). Fourier bases are usually used for data with a repetitive pattern and B-splines functions for smooth curves (Schmutz et al, 2020). The number of basis functions depends on the data and can be chosen using cross-validation.

3.1 The functional latent mixture model

We assume that for every $k \in \{1, \dots, K\}$ the stochastic process $\mathbf{X}$ associated with the k th cluster can be described in a lower dimensional subspace $\mathbb{E}^k[0, \mathcal{T}_X] \subset L^2[0, \mathcal{T}_X]$ with dimension $d_k \leq R^X$ and spanned by the first d_k elements of a group specific basis of functions $\{\zeta_{X,kr}, r = 1, \dots, R^X\}$ that can be obtained from $\{\xi_{X,r}^l, l = 1, \dots, p_X, r = 1, \dots, R^X\}$ by a linear transformation using a MFPCA such that we have

$$\zeta_{X,kr}(t) = \sum_{j=1}^{R^X} q_{krj} \xi_{X,j}(t), \quad r = 1, \dots, R^X,$$

where $\mathbf{Q}_k = (q_{krj})_{r,j=1,\dots,R^X}$ is the orthogonal $R^X \times R^X$ matrix containing the coefficients of the eigenfunctions expressed in the initial basis $\boldsymbol{\xi}$. Using (6) the MFPCA scores can be obtained directly from a principal component analysis of the coefficients $\mathbf{C}_X$ with a metric based on the inner products between the basis functions included in $\mathbf{W}_X$. We suppose that the first d_k eigenfunctions contain the main information of the MFPCA of cluster k and we split $\mathbf{Q}_k = [\mathbf{U}_k, \mathbf{V}_k]$ such that $\mathbf{U}_k$ is of size $R^X \times d_k$, $\mathbf{V}_k$ is of size $R^X \times (R^X - d_k)$ and we have

$$\mathbf{Q}_k^\top \mathbf{Q}_k = \mathbf{I}_{R^X}, \quad \mathbf{U}_k^\top \mathbf{U}_k = \mathbf{I}_{d_k}, \quad \mathbf{V}_k^\top \mathbf{V}_k = \mathbf{I}_{R^X - d_k}, \quad \mathbf{U}_k^\top \mathbf{V}_k = \mathbf{0}.$$

The relationship between the column vector formed with the coefficients $\mathbf{c}_{X,i}$ in the i th row of the matrix $\mathbf{C}_X$ and the score δ_i is

$$\mathbf{c}_{X,i} = \mathbf{W}_X^{-1/2} \mathbf{U}_k \delta_i + \mathbf{e}_i,$$

where $\mathbf{e}_i$ is the noise.

We can make distribution assumptions on the scores δ_i (Delaigle and Hall, 2010), so, as for the model associated with the funHDDC method (Schmutz et al, 2020), we assume that independently for $i = 1, \dots, n$

$$\mathbf{e}_i \mid Z_{ik} = 1 \sim N(\mathbf{0}, \mathbf{\Lambda}_k), \text{ and } \delta_i \mid Z_{ik} = 1 \sim N(\mathbf{m}_k, \mathbf{\Delta}_k).$$

Thus

$$\mathbf{c}_{X,i} \mid Z_{ik} = 1 \sim N(\boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k}). \quad (13)$$

Let $\phi(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k})$ denotes the density for the R_X -variate normal distribution $N(\boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k})$

$$\phi(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k}) = (2\pi)^{-R_X/2} |\boldsymbol{\Sigma}_{X,k}|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1}(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})\right). \quad (14)$$

Here $|\boldsymbol{\Sigma}_{X,k}|$ denotes the determinant of $\boldsymbol{\Sigma}_{X,k}$, and

$$\boldsymbol{\mu}_{X,k} = \mathbf{W}_X^{-1/2} \mathbf{U}_k \mathbf{m}_k, \quad \boldsymbol{\Sigma}_{X,k} = \mathbf{W}_X^{-1/2} \mathbf{U}_k \boldsymbol{\Delta}_k \mathbf{U}_k^\top \mathbf{W}_X^{-1/2} + \boldsymbol{\Lambda}_k, \quad (15)$$

where the noise covariance $\boldsymbol{\Lambda}_k$ is such that the covariance $\mathbf{D}_k$ of the data in the space generated by the eigenfunctions $\boldsymbol{\zeta}_{X,kr}$ is a diagonal matrix given by

$$\mathbf{D}_k = \mathbf{Q}_k^\top \mathbf{W}_X^{1/2} \boldsymbol{\Sigma}_{X,k} \mathbf{W}_X^{1/2} \mathbf{Q}_k = \text{diag}(a_{k1}, \dots, a_{kd_k}, b_k, \dots, b_k), \quad (16)$$

with $a_{k1} > a_{k2} > \dots > a_{kd_k} > b_k$.

Given that $Z_{ik} = 1$, from (12) we have for the column vector formed with the coefficients $\mathbf{c}_{Y,i}$ in the i th row of the matrix $\mathbf{C}_Y$:

$$\mathbf{c}_{Y,i} = \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* + \boldsymbol{\epsilon}_0^k,$$

where $\mathbf{c}_{X,i}^* = \begin{pmatrix} \mathbf{W}_X \mathbf{c}_{X,i} \\ 1 \end{pmatrix}$ and $\boldsymbol{\Gamma}_*^k$ is the $R_Y \times (R_X + 1)$ matrix $\boldsymbol{\Gamma}_*^k = (\boldsymbol{\Gamma}^k, \boldsymbol{\Gamma}_0^k)$. Thus

$$\mathbf{c}_{Y,i} \mid Z_{ik} = 1, \mathbf{c}_{X,i} \sim N(\boldsymbol{\mu}_{Y,k}, \boldsymbol{\Sigma}_{Y,k}), \quad \boldsymbol{\mu}_{Y,k} = \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* \quad (17)$$

Thus the joint distribution of the coefficients $(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i})$, $i = 1, \dots, n$ arise from a parametric mixture distribution

$$p(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i}; \boldsymbol{\theta}) = \sum_{k=1}^K \pi_k p_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k), \quad \sum_{k=1}^K \pi_k = 1, \quad (18)$$

$$p_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k) = f_k(\mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k) g_k(\mathbf{c}_{Y,i} \mid \mathbf{c}_{X,i}, \boldsymbol{\theta}_k), \quad (19)$$

where $\pi_k \in (0, 1]$ are the mixing proportions, $\boldsymbol{\theta}_k = \{\boldsymbol{\mu}_{X,k}, a_{kj}, b_k, \mathbf{q}_{kj}, \boldsymbol{\Sigma}_{Y,k}, \boldsymbol{\Gamma}_*^k\}$ and $\boldsymbol{\theta} = \bigcup_{k=1}^K (\boldsymbol{\theta}_k \cup \{\pi_k\})$, is the set formed with the parameters. Here $f_k(\mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k) = \phi(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k})$ is given in (14), and $g_k(\mathbf{c}_{Y,i} \mid \mathbf{c}_{X,i}, \boldsymbol{\theta}_k)$ is the conditional density of the multivariate response $\mathbf{c}_{Y,i}$ given the covariates $\mathbf{c}_{X,i}$ and $Z_{ik} = 1$. From (17) we have $g_k(\mathbf{c}_{Y,i} \mid \mathbf{c}_{X,i}, \boldsymbol{\theta}_k) = \phi(\mathbf{c}_{Y,i}; \boldsymbol{\mu}_{Y,k}, \boldsymbol{\Sigma}_{Y,k})$.

As in Schmutz et al (2020) we refer to this model for $\mathbf{X}$ as FLM $[a_{kj}, b_k, \mathbf{Q}_k, d_k]$ (functional latent mixture) and we consider the parsimonious sub-models:

- FLM $[a_{kj}, b, \mathbf{Q}_k, d_k]$: the parameters b_k are common between the clusters

- FLM[$a_k, b_k, \mathbf{Q}_k, d_k$]: the first d_k diagonal elements of $\mathbf{D}_k$ are common within each class
- FLM[$a, b_k, \mathbf{Q}_k, d_k$]: the first d_k diagonal elements of $\mathbf{D}_k$ are common within each class and between the clusters
- FLM[$a_k, b, \mathbf{Q}_k, d_k$]: the parameters b_k are common between the clusters and the first d_k diagonal elements of $\mathbf{D}_k$ are common within each class
- FLM[$a, b, \mathbf{Q}_k, d_k$]: the parameters b_k are common between the clusters and the first d_k diagonal elements of $\mathbf{D}_k$ are common within each class and between the clusters

Table 1 Number of free parameters for the FLM models

Model	Number of free parameters	Model	Number of free parameters
FLM[$a_{kj}, b_k, \mathbf{Q}_k, d_k$]	$\tau_1 + \tau_2 + 2K + \sum_{k=1}^K d_k$	FLM[$a, b_k, \mathbf{Q}_k, d_k$]	$\tau_1 + \tau_2 + 2K + 1$
FLM[$a_{kj}, b, \mathbf{Q}_k, d_k$]	$\tau_1 + \tau_2 + K + 1 + \sum_{k=1}^K d_k$	FLM[$a_k, b, \mathbf{Q}_k, d_k$]	$\tau_1 + \tau_2 + 2K + 1$
FLM[$a_k, b_k, \mathbf{Q}_k, d_k$]	$\tau_1 + \tau_2 + 3K$	FLM[$a, b, \mathbf{Q}_k, d_k$]	$\tau_1 + \tau_2 + K + 2$

Next we analyze the complexity of the FLM models. Let $\tau_1 = KR_X + K - 1$ be the number of parameters required for the estimation of the means μ_k and the proportions π_k and $\tau_2 = \sum_{k=1}^K d_k[R_X - (d_k + 1)/2]$ be the number of parameters required for the estimation of the matrices $\mathbf{Q}_k$. Adding also the number of parameters required for the estimation of b_k, a_{kj} , and d_k gives the total number of parameters to be estimated as included in Table 1 (see also Table 1 in Bouveyron and Jacques (2011)).

Table 2 Parsimonious models and the number of free parameters for the eigen-decomposed $\Sigma_{Y,k}$

Model	$\Sigma_{Y,k}$	Number of free parameters for $\Sigma_{Y,k}$
EII	$\lambda \mathbf{I}_{R^Y}$	1
VII	$\lambda_k \mathbf{I}_{R^Y}$	K
E EI	$\lambda \Upsilon$	R^Y
VEI	$\lambda_k \Upsilon$	$K + R^Y - 1$
EVI	$\lambda \Upsilon_k$	$K R^Y - (K - 1)$
VVI	$\lambda_k \Upsilon_k$	$K R^Y$
EEE	$\lambda \Xi \Upsilon \Xi^\top$	$R^Y(R^Y + 1)/2$
VEE	$\lambda_k \Xi \Upsilon \Xi^\top$	$R^Y(R^Y + 1)/2 + K - 1$
EVE	$\lambda \Xi \Upsilon_k \Xi^\top$	$R^Y(R^Y + 1)/2 + (K - 1)(R^Y - 1)$
EEV	$\lambda \Xi_k \Upsilon \Xi_k^\top$	$K R^Y(R^Y + 1)/2 - (K - 1)R^Y$
VVE	$\lambda_k \Xi \Upsilon_k \Xi_k^\top$	$R^Y(R^Y + 1)/2 + (K - 1)R^Y$
VEV	$\lambda_k \Xi_k \Upsilon \Xi_k^\top$	$K R^Y(R^Y + 1)/2 - (K - 1)(R^Y - 1)$
EVV	$\lambda \Xi_k \Upsilon_k \Xi_k^\top$	$K R^Y(R^Y + 1)/2 - (K - 1)$
VVV	$\lambda_k \Xi_k \Upsilon_k \Xi_k^\top$	$K R^Y(R^Y + 1)/2$

As in [Celeux and Govaert \(1995\)](#) we consider parsimony also for the matrices $\Sigma_{Y,k}$. An eigen-decomposition gives $\Sigma_{Y,k} = \lambda_k \Xi_k \Upsilon_k \Xi_k^\top$, where $\lambda_k = |\Sigma_{Y,k}|^{1/R^Y}$ is a constant, Υ_k is a diagonal matrix with entries (sorted in decreasing order) proportional to the eigenvalues of $\Sigma_{Y,k}$ with the constraint $|\Upsilon_k| = 1$, and Ξ_k is a $R^Y \times R^Y$ orthogonal matrix of the eigenvectors (ordered according to the eigenvalues) of $\Sigma_{Y,k}$, $k = 1, \dots, K$. We get the models in Table 2.

We denote a combination between a FLM[$a_{kj}, b_k, \mathbf{Q}_k, d_k$] model and a VVV covariance structure as a FLM[$a_{kj}, b_k, \mathbf{Q}_k, d_k$] - VVV model. We have $6 \times 14 = 84$ parsimonious models. The number of parameters τ to be estimated for these models is equal with the sum between the parameters coming from the FLM model (see Table 1) and the parameters pertaining to the model for the covariance structure (see the last column in Table 2).

3.2 Model Identifiability

Before presenting an EM algorithm for parameter estimation, it is important to study identifiability. Identifiability of the functional model (7), reduces to the identifiability of the model (18)-(19) in the space of the coefficients, which, roughly speaking, means that two sets of parameters φ and $\tilde{\varphi}$ that do not agree after permutation cannot give the same mixture distribution.

Identifiability of multivariate finite Gaussian mixture distributions is shown in [Yakowitz and Spragins \(1968\)](#), and general conditions for identifiability of mixture of linear models are given in [Hennig \(2000\)](#). Here we study the identifiability of the most general model FLM[$a_{kj}, b_k, \mathbf{Q}_k, d_k$] - VVV following the approach used in [Dang et al \(2017\)](#), where a sufficient identification condition is provided for the CWM with multivariate correlated responses given in (1).

We define the parametric class of probability density functions

$$\begin{aligned} \mathcal{C} := & \left\{ p(\mathbf{c}_Y, \mathbf{c}_X; \varphi) = \sum_{k=1}^K \pi_k \phi(\mathbf{c}_Y; \Gamma_*^k \mathbf{c}_X^*, \Sigma_{Y,k}) \phi(\mathbf{c}_X; \mu_{X,k}, \Sigma_{X,k}), \text{ with } \pi_k > 0, \right. \\ & \sum_{k=1}^K \pi_k = 1, (\Gamma_*^k, \Sigma_{Y,k}) \neq (\Gamma_*^i, \Sigma_{Y,i}), \text{ for } i \neq k, \mathbf{c}_Y \in \mathbb{R}^{R^Y}, \mathbf{c}_X \in \mathbb{R}^{R^X}, \mathbf{c}_X^* = \begin{pmatrix} \mathbf{W}_X \mathbf{c}_X \\ 1 \end{pmatrix}, \\ & \left. \varphi = \left\{ \Gamma_*^k, \Sigma_{Y,k}, \mu_{X,k}, \Sigma_{X,k}, \pi_k : k = 1, \dots, K \right\}, K \in \mathbb{N} \right\} \end{aligned}$$

The next theorem proves that for $p(\mathbf{c}_Y, \mathbf{c}_X; \varphi), p(\mathbf{c}_Y, \mathbf{c}_X; \tilde{\varphi}) \in \mathcal{C}$,

$$\begin{aligned} p(\mathbf{c}_Y, \mathbf{c}_X; \varphi) &= \sum_{k=1}^K \pi_k \phi(\mathbf{c}_Y; \Gamma_*^k \mathbf{c}_X^*, \Sigma_{Y,k}) \phi(\mathbf{c}_X; \mu_{X,k}, \Sigma_{X,k}), \\ p(\mathbf{c}_Y, \mathbf{c}_X; \tilde{\varphi}) &= \sum_{k=1}^{\tilde{K}} \tilde{\pi}_k \phi(\mathbf{c}_Y; \tilde{\Gamma}_*^k \mathbf{c}_X^*, \tilde{\Sigma}_{Y,k}) \phi(\mathbf{c}_X; \tilde{\mu}_{X,k}, \tilde{\Sigma}_{X,k}), \end{aligned}$$

we have $p(\mathbf{c}_Y, \mathbf{c}_X; \boldsymbol{\varphi}) = p(\mathbf{c}_Y, \mathbf{c}_X; \tilde{\boldsymbol{\varphi}})$ for almost all $\mathbf{c}_X \in \mathbb{R}^{R_X}$ and for all $\mathbf{c}_Y \in \mathbb{R}^{R_Y}$ if and only if $K = \tilde{K}$, and for each $k \in \{1, \dots, K\}$ there exists $i \in \{1, \dots, K\}$ such that $\mathbf{\Gamma}_*^k = \tilde{\mathbf{\Gamma}}_*^i$, $\mathbf{\Sigma}_{Y,k} = \tilde{\mathbf{\Sigma}}_{Y,i}$, $\boldsymbol{\mu}_{X,k} = \tilde{\boldsymbol{\mu}}_{X,i}$, $\mathbf{\Sigma}_{X,k} = \tilde{\mathbf{\Sigma}}_{X,i}$, and $\pi_k = \tilde{\pi}_i$.

Theorem 1. Suppose that there exists a set $\mathcal{X} \in \mathbb{R}^{R_X}$ having probability equal to one according to the R_X -variate Gaussian distribution such that the mixture of regression models

$$\sum_{k=1}^K \phi(\mathbf{c}_Y; \mathbf{\Gamma}_*^k \mathbf{c}_X^*, \mathbf{\Sigma}_{Y,k}) \alpha_k(\mathbf{c}_X), \quad \mathbf{c}_Y \in \mathbb{R}^{R_Y},$$

is identifiable for each fixed $\mathbf{c}_X \in \mathcal{X}$, where $\alpha_k(\mathbf{c}_X) > 0$, $k = 1, \dots, K$, $\sum_{k=1}^K \alpha_k(\mathbf{c}_X) = 1$ for each $\mathbf{c}_X \in \mathcal{X}$. Then the class $\mathcal{C}$ is identifiable in $\mathcal{X} \times \mathbb{R}^{R_Y}$.

Proof. The proof is similar the proof of Theorem 1 in [Dang et al \(2017\)](#). □

4 Learning the FLM[a_{kj}, b_k, Q_k, d_k] - VVV model

To fit the models, we use the expectation-maximization (EM) algorithm ([Dempster et al, 1977](#)). The algorithm consists of successive iterations of the expectation (E) and the maximization (M) steps until convergence is achieved. The clusters' labels $\mathbf{Z}_i$ are the missing data, so the complete data are given by $\{\mathbf{c}_{Y,i}, \mathbf{c}_{X,i}, z_{ik}, i = 1, \dots, n, k = 1, \dots, K\}$. The current estimates of the parameters are used in the E step to compute the conditional expectation of the complete log-likelihood. In the M step the estimates of the parameters are updated with the values that maximize the expected complete log-likelihood. Next we present the EM algorithm for the most general model FLM[a_{kj}, b_k, Q_k, d_k] - VVV model. The main steps of the proposed EM algorithm are summarized in Algorithm 1.

Proposition 2. The complete data log-likelihood of the observed curves under the FLM[a_{kj}, b_k, Q_k, d_k] - VVV model for $\mathbf{X}$ can be written as

$$l_c(\boldsymbol{\theta}) = l_{1c}(\pi) + l_{2c}(\boldsymbol{\vartheta}_X) + l_{3c}(\boldsymbol{\vartheta}_Y) \quad (20)$$

where

$$l_{1c}(\pi) = \sum_{i=1}^n \sum_{k=1}^K z_{ik} \log(\pi_k), \quad (21)$$

$$\begin{aligned} l_{2c}(\boldsymbol{\vartheta}_X) = & -\frac{nR_X \log(2\pi)}{2} + \frac{n}{2} \log(|\mathbf{W}_X|) - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=1}^{d_k} \log(a_{kl}) \\ & - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=d_k+1}^{R_X} \log(b_k) - \frac{1}{2} \sum_{k=1}^K \left(\sum_{l=1}^{d_k} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{a_{kl}} \right. \\ & \left. + \sum_{l=d_k+1}^R \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{b_k} \right) \end{aligned} \quad (22)$$

$$l_{3c}(\boldsymbol{\vartheta}_Y) = -\frac{nR_Y \log(2\pi)}{2} - \frac{n}{2} \sum_{k=1}^K n_k \log |\boldsymbol{\Sigma}_{Y,k}| - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K z_{ik} \left(\mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} \right. \\ \left. - \mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* - (\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} + (\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* \right) \quad (23)$$

where $\boldsymbol{\vartheta}_X = \{\boldsymbol{\mu}_{X,k}, a_{kj}, b_k, \mathbf{q}_{kj}\}$, $\boldsymbol{\vartheta}_Y = \{\boldsymbol{\Sigma}_{Y,k}, \boldsymbol{\Gamma}_*^k\}$, $k = 1, \dots, K$, $j = 1, \dots, d_k$, with $\mathbf{q}_{kj}$ the j th column of $\mathbf{Q}_k$, $n_k = \sum_{i=1}^n z_{ik}$, and $\mathbf{S}_{X,k}$ is defined by

$$\mathbf{S}_{X,k} := \sum_{i=1}^n z_{ik} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top. \quad (24)$$

Proof. The proof is included in Appendix A. $\square$

4.0.1 The E-step

At the m th iteration of the EM algorithm we calculate $E[l_c(\boldsymbol{\theta}^{(m-1)}) \mid \mathbf{c}_{Y,1}, \mathbf{c}_{X,1}, \dots, \mathbf{c}_{Y,n}, \mathbf{c}_{X,n}, \boldsymbol{\theta}^{(m-1)}]$, given the current values of the parameters $\boldsymbol{\theta}^{(m-1)}$. This reduces to the calculation of $E[Z_{ik} \mid \mathbf{c}_{Y,1}, \mathbf{c}_{X,1}, \dots, \mathbf{c}_{Y,n}, \mathbf{c}_{X,n}, \boldsymbol{\theta}^{(m-1)}]$.

Proposition 3. *Let us denote*

$$H_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k) := -2 \log(\pi_k) + \sum_{j=1}^{d_k} \log(a_{kj}) + (R_X - d_k) \log(b_k) \\ + \log(|\boldsymbol{\Sigma}_{Y,k}|) + \delta(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \mathbf{Q}_k, a, b, d_k) + (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \\ (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*) \quad (25)$$

$$\delta(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \mathbf{Q}_k, a, b, d_k) := \sum_{l=1}^{d_k} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{a_{kl}} \\ + \sum_{l=d_k+1}^p \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{b_k} \quad (26)$$

We have

$$t_{ik}^{(m)} := E[Z_{ik} \mid \mathbf{c}_{Y,1}, \mathbf{c}_{X,1}, \dots, \mathbf{c}_{Y,n}, \mathbf{c}_{X,n}, \boldsymbol{\theta}^{(m-1)}] = \frac{\pi_k p_k \left(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k^{(m-1)} \right)}{\sum_{l=1}^K \pi_l p_l \left(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_l^{(m-1)} \right)} \\ = \frac{1}{\sum_{l=1}^K \exp \left(\frac{1}{2} \left(H_k \left(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k^{(m-1)} \right) - H_l \left(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_l^{(m-1)} \right) \right) \right)}, \quad (27)$$

Proof. The proof is included in Appendix B. $\square$

Based on the current values of the parameters $\boldsymbol{\theta}^{(m-1)}$ the log-likelihood is given by

$$\begin{aligned}\mathbb{L}^{(m-1)} &= \log \left(\prod_{i=1}^n p(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i}; \boldsymbol{\theta}^{(m-1)}) \right) \\ &= \sum_{i=1}^n \log \left(\sum_{k=1}^K \pi_k^{(m-1)} p_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k^{(m-1)}) \right)\end{aligned}$$

4.0.2 The M-step

In the M-step at the m th iteration of the EM algorithm we estimate the parameters by maximizing the conditional expectation of the complete data log likelihood $Q(\boldsymbol{\theta} \mid \boldsymbol{\theta}^{(m-1)}) := E[\log(l_c(\boldsymbol{\theta}^{(m-1)})) \mid \mathbf{c}_{Y,1}, \mathbf{c}_{X,1}, \dots, \mathbf{c}_{Y,n}, \mathbf{c}_{X,n}, \boldsymbol{\theta}^{(m-1)}]$.

Proposition 4. *Let*

$$\mathbf{S}_{X,k}^{(m)} = \frac{\sum_{i=1}^n t_{ik}^{(m)} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}^{(m)}) (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}^{(m)})^\top}{n_k^{(m)}}, \quad n_k^{(m)} = \sum_{i=1}^n t_{ik}^{(m)}. \quad (28)$$

For the model $FLM[a_{kj}, b_k, \mathbf{Q}_k, d_k]$ -VWV we have the following updates for the parameters, $k = 1, \dots, K$

$$\pi_k^{(m)} = \frac{\sum_{i=1}^n t_{ik}^{(m)}}{n} = \frac{n_k^{(m)}}{n}, \quad (29)$$

$$\boldsymbol{\mu}_{X,k}^{(m)} = \frac{\sum_{i=1}^n t_{ik}^{(m)} \mathbf{c}_{X,i}}{\sum_{i=1}^n t_{ik}^{(m)}} \quad (30)$$

$$(\boldsymbol{\Gamma}_*^k)^{(m)} = \left(\sum_{i=1}^n t_{ik}^{(m)} \mathbf{c}_{Y,i} (\mathbf{c}_{X,i}^*)^\top \right) \left(\sum_{i=1}^n t_{ik}^{(m)} \mathbf{c}_{X,i}^* (\mathbf{c}_{X,i}^*)^\top \right)^{-1}, \quad (31)$$

$$\boldsymbol{\Sigma}_{Y,k}^{(m)} = \frac{\sum_{i=1}^n t_{ik}^{(m)} (\mathbf{c}_{Y,i} - (\boldsymbol{\Gamma}_*^k)^{(m)} \mathbf{c}_{X,i}^*) (\mathbf{c}_{Y,i} - (\boldsymbol{\Gamma}_*^k)^{(m)} \mathbf{c}_{X,i}^*)^\top}{n_k^{(m)}}. \quad (32)$$

- $\mathbf{q}_{kj}^{(m)}$, $k = 1, \dots, K, j = 1, \dots, d_k$ are updated as the eigenfunctions associated with the d_k largest eigenvalues of $\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}$;
- $a_{kj}^{(m)}$, $k = 1, \dots, K, j = 1, \dots, d_k$ are updated by the d_k largest eigenvalues of $\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}$;
- $b_k^{(m)}$, $k = 1, \dots, K$ are updated by

$$b_k^{(m)} = \frac{1}{R_X - d_k} \left(\text{trace} \left(\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \right) - \sum_{j=1}^{d_k} a_{kj}^{(m)} \right). \quad (33)$$

Proof. The proof is included in Appendix C. $\square$

For the other parsimonious models the updates in the M-step are different only for the covariance matrix $\Sigma_{Y,k}^{(m)}$ and $a_{kj}^{(m)}, b_k^{(m)}, k = 1, \dots, K, j = 1, \dots, d_k$. For the models in Table 2 for the covariance matrix $\Sigma_{Y,k}^{(m)}$ the updates are similar with those of the Gaussian parsimonious clustering models in Celeux and Govaert (1995). For the simplified FLM models we have:

- FLM[$a_{kj}, b, \mathbf{Q}_k, d_k$] for $\mathbf{X}$: the estimator of b is

$$b^{(m)} = \frac{\text{trace} \left(\sum_{k=1}^K \pi_k^{(m)} \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \right) - \sum_{k=1}^K \pi_k^{(m)} \sum_{j=1}^{d_k} a_{kj}^{(m)}}{R_X - \sum_{k=1}^K \pi_k^{(m)} d_k} \quad (34)$$

- FLM[$a_k, b_k, \mathbf{Q}_k, d_k$] for $\mathbf{X}$: the estimator of a_k is

$$a_k^{(m)} = \frac{\sum_{j=1}^{d_k} a_{kj}^{(m)}}{d_k} \quad (35)$$

and the estimator of b_k is given by (33).

- FLM[$a, b_k, \mathbf{Q}_k, d_k$] for $\mathbf{X}$: the estimator of a is

$$a^{(m)} = \frac{\sum_{k=1}^K \pi_k^{(m)} \sum_{j=1}^{d_k} a_{kj}^{(m)}}{\sum_{k=1}^K \pi_k^{(m)} d_k} \quad (36)$$

and the estimator of b_k is given by (33).

- FLM[$a_k, b, \mathbf{Q}_k, d_k$] for $\mathbf{X}$: the estimator of a_k is given by (35) and the estimator of b is given by (34).
- FLM[$a, b, \mathbf{Q}_k, d_k$] for $\mathbf{X}$: the estimator of a is given by (36) and the estimator of b is given by (34).

4.0.3 Initialization

To start the EM algorithm, we need initial values $t_{ik}^{(0)}$. As for funHDDC (Schmutz et al, 2020), we have implemented a random initialization and an initialization with the *kmeans* method available in the *stats* package in R. For random initialization, the values of $t_{ik}^{(0)}$ correspond to a partition randomly sampled using a multinomial distribution with uniform probabilities. For the *kmeans* strategy, the values of $t_{ik}^{(0)}$ correspond to the partition obtained applying the *kmeans* method to the data set formed by the combining the coefficients $\mathbf{C}_X, \mathbf{C}_Y$.

To prevent the convergence of the EM algorithm to a local maximum, we execute the algorithm with different initialization values for $t_{ik}^{(0)}$, and we keep the best result given by the EM algorithm using the Bayesian information criterion (BIC; Schwarz, 1978) defined by

$$BIC = L^{(m_f)} - \frac{\tau}{2} \log n, \quad (37)$$

Algorithm 1 EM algorithm for funWeightClust

Input: data $(\mathbf{y}_1, \mathbf{x}_1), \dots, (\mathbf{y}_n, \mathbf{x}_n)$, range for number of clusters $K = K_1, \dots, K_G$, funWeightClust models set_{models} , initialization method $init \in \{kmeans, random\}$, number of repetitions for initialization n_{rep} , threshold for Cattell scree-test ϵ , maximum number of iterations max_{iter} , precision ϵ_1

```
1: Compute  $W_X$  and  $W_X^{1/2}$ 
2: for  $K = K_1$  to  $K_G$  do (this can be performed in parallel)
3:   for  $r = 1$  to  $n_{rep}$  do (this can be performed in parallel)
4:     Initialization
5:     Apply method  $init$  to calculate  $t_{ik}^{(0)}$ ,  $i = 1, \dots, n$ ,  $k = 1, \dots, K$ 
6:     for all  $model \in set_{models}$  do
7:        $m \leftarrow 1$ 
8:        $test \leftarrow \epsilon_1 + 1$ 
9:       while  $m \leq max_{iter}$  and  $test \geq \epsilon_1$  do
10:        M-step
11:        Compute  $d_k^{(m)}$  using Cattell scree test with threshold  $\epsilon$ ,
12:         $k = 1, \dots, K$ 
13:        Compute  $\theta^{(m)} = \{\pi_k^{(m)}, \mu_{X,k}^{(m)}, a_{kj}^{(m)}, b_k^{(m)}, q_{kj}^{(m)}, \Sigma_{Y,k}^{(m)}, (\Gamma_*^k)^{(m)}\}$ ,
14:         $k = 1, \dots, K$ ,  $j = 1, \dots, d_k^{(m)}$ 
15:        E-step
16:        Compute  $t_{ik}^{(m)}$ ,  $i = 1, \dots, n$ ,  $k = 1, \dots, K$ 
17:        Compute the log likelihood  $L^{(m)}$ 
18:        if  $m = 2$  then
19:           $test \leftarrow L^{(m)} - L^{(m-1)}$ 
20:        end if
21:        if  $m > 2$  then
22:          Compute Aitken acceleration  $A \leftarrow \frac{L^{(m)} - L^{(m-1)}}{L^{(m-1)} - L^{(m-2)}}$ 
23:          Compute the asymptotic estimate  $AL \leftarrow L^{(m-1)} + \frac{L^{(m)} - L^{(m-1)}}{1 - A}$ 
24:          Compute  $test \leftarrow |AL - L^{(m-1)}|$ 
25:        end if
26:      end while
27:      Compute BIC
28:      Assign a cluster to each observation  $(\mathbf{y}_i, \mathbf{x}_i)$ ,  $i = 1, \dots, n$  using MAP
29:    end for
30:  end for
31:  Choose the model with the maximum BIC if the number of clusters is  $K$ 
32: end for
33: Choose the number of clusters  $K$  that gives the largest BIC
```

Output: the best number of clusters, the best model, the assigned clusters

where τ is the overall number of the free parameters, n is the number of observations, $L^{(m_f)}$ is the maximum log-likelihood value, and m_f is the last iteration of the algorithm

before convergence. For the numerical experiments in Section 5 we consider the number of initializations to be at least 20.

4.0.4 Estimation of the hyper-parameters, convergence criterion, and the classification step

The number of clusters K and the parsimonious model are selected by maximizing the the BIC given in (37). The group specific dimension d_k is selected through the Cattell scree-test by comparison of the difference between eigenvalues with a given threshold ϵ (Bouveyron and Jacques, 2011). In Amovin-Assagba et al (2022) a grid search is applied and d_k is chosen as the positive integer from the grid that corresponds to the maximum value of the BIC. Since the grid search requires substantially more time and we have not obtained a major improvement using the grid search, in Section 5 we present the results obtained with the Cattell scree-test.

To avoid spurious clusters, which are a known problem for mixture models (McLachlan and Peel, 2004), we proceed as in Dang et al (2017) and we remove the models that have a matrix $\Sigma_{Y,k}^{(m_f)}$ for which at least one eigenvalue is less than 10^{-20} . In the simulations presented in section 5.1 this procedure has the effect of disregarding all models with spurious clusters and obtaining more accurate estimations for the number of clusters K .

We consider that the EM algorithm has converged if a maximum number of iterations is reached or $|L_\infty^{(m+2)} - L^{(m+1)}| < \epsilon_1$ (McNicholas et al, 2010), where $L^{(m+1)}$ is the log-likelihood value at iteration $m+1$, and $L_\infty^{(m+2)}$ is the asymptotic estimate of log-likelihood at iteration $m+2$ (Andrews et al, 2011) defined as

$$L_\infty^{(m+2)} = L^{(m+1)} + \frac{L^{(m+2)} - L^{(m+1)}}{1 - a^{(m+1)}}.$$

Here $a^{(m+1)}$ is the Aitken acceleration (Aitken, 1927) at iteration $m+1$:

$$a^{(m+1)} = \frac{L^{(m+2)} - L^{(m+1)}}{L^{(m+1)} - L^{(m)}}$$

We choose 200 for the maximum number of iterations and the precision $\epsilon_1 = 10^{-6}$.

We determine the clusters using the maximum *a posteriori* (MAP) rule: an observation $(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i})$ is assigned to the cluster $k \in \{1, \dots, K\}$ with the largest $t_{ik}^{(m_f)}$, where m_f is the last iteration of the EM algorithm before convergence.

5 Experiments and results

We apply the proposed clustering method to simulated data, the Adelaide electricity demand data (available in the *fds* package in R), and Edmonton traffic data. For some of these clustering examples, the true classifications are known and the Adjusted Rand Index (ARI; Hubert and Arabie, 1985) is used to measure the accuracy of the classification. The expected value of the adjusted Rand index is 0, and for a perfect

classification its value is 1. Negative values for ARI indicates that the classification is worse than would be expected by random assignment. We compare `funWeightClust` with methods for clustering functional data (*funHDDC* R package) and methods for clustering multivariate data (*flexmix* and *mclust* R packages). When we apply the methods for clustering multivariate data we use the two approaches mentioned at the beginning of section 2: a raw-data clustering and a two-step method.

5.1 Simulation studies on synthetic data sets

We simulate 600 pairs of curves according to the $FLM[a_{kj}, b_k, \mathbf{Q}_k, d_k] \times VII$ model. The number of clusters is 2 and the mixing proportions are $\pi_1 = \pi_2 = 1/2$. We consider two scenarios. For the first scenario for the covariates curves X_i the parameters are

$$\begin{aligned} \text{Group 1: } d_1 &= 2, \mathbf{a}_1 = (6730.074, 1641.839)^\top, b_1 = 70.57964, \boldsymbol{\mu}_{X,1} = \\ &= (1459.420, 1297.329, 883.6936, 1052.785, 1167.558, 1183.825)^\top \\ \text{Group 2: } d_2 &= 1, a_2 = 95464.836, b_2 = 2351.284, \boldsymbol{\mu}_{X,2} = \\ &= (1555.634, 1450.803, 867.3406, 1429.287, 1528.500, 1517.618)^\top \end{aligned}$$

where d_k is the intrinsic dimension of the subgroups, $\boldsymbol{\mu}_{X,k}$ is the mean vector of size 6, $\mathbf{a}_k$ includes the values of the d_k -first diagonal elements of $\mathbf{D}$, and b_k the value of the last $6 - d_k$ - elements, $k = 1, 2$. Curves are smoothed using 6 cubic B-spline basis functions. For the response curves Y_i the coefficients are generated using the coefficients of the curves X_i and equation (12) with the values of regression coefficients $\boldsymbol{\Gamma}^1, \boldsymbol{\Gamma}^2, \boldsymbol{\Gamma}_0^1, \boldsymbol{\Gamma}_0^2$ given in Appendix D, and $\boldsymbol{\Sigma}_{Y,1} = 434.6492 \mathbf{I}_6$, $\boldsymbol{\Sigma}_{Y,2} = 1014.901 \mathbf{I}_6$, where $\mathbf{I}_6$ is the 6th dimensional identity matrix. Curves are smoothed using 6 cubic B-spline basis functions.

We can notice in Figure 2 that while the Y_i curves from the two clusters overlap, there is a visible separation between the clusters for the X_i curves. We also simulate the more difficult scenario illustrated in Figure 3. The parameters are the same as before except the values for $\boldsymbol{\mu}_{X,k}$, $k = 1, 2$:

$$\begin{aligned} \text{Group 1: } \boldsymbol{\mu}_{X,1} &= (1042.4431, 926.6636, 631.2097, 751.9895, 833.9701, 845.5891)^\top \\ \text{Group 2: } \boldsymbol{\mu}_{X,2} &= (1111.167, 1036.288, 619.529, 1020.919, 1091.786, 1084.013)^\top \end{aligned}$$

For both scenarios we repeat the simulation 100 times. We use ARI to evaluate the clustering done with `funWeightClust` and `funHDDC`. We apply `funHDDC` for the curves obtained by combining the $X_i : [0, 12] \rightarrow \mathbb{R}$ and $Y_i : [12, 24] \rightarrow \mathbb{R}$ curves in one curve over the time interval $[0, 24]$. Alternatively, we consider the pairs of curves (X_i, Y_i) as two-dimensional functional data when we apply `funHDDC`. We run `funWeightClust` and `funHDDC` for $K = 2$ with all sub-models, and the best solution in terms of the highest BIC value for all those sub-models is returned. The initialization is done with the *kmeans* method with 50 repetitions, and the maximum number of iterations is 200 for the stopping criterion. We use $\epsilon \in \{0.005, 0.01, 0.2\}$ in the Cattell test. We denote the method applied to the combined curves by `funHDDC`, and we denote `funHDDC` applied to the two-dimensional curves (X_i, Y_i) by `2D-funHDDC`.

From the results included in Table 3 we notice that `funWeightClust` outperforms `funHDDC` and `2D-funHDDC`. For scenario 1 both `funHddc` and `funWeightClust` give

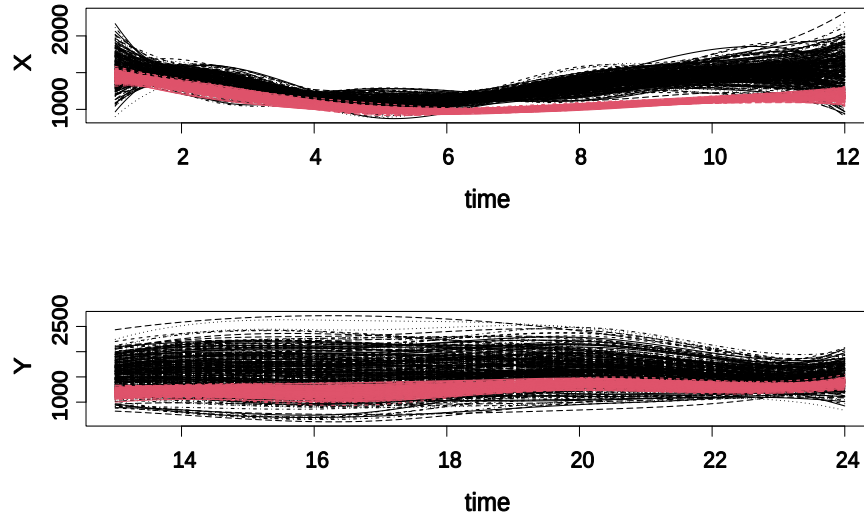


Fig. 2 Smooth data simulated according to scenario 1 colored by group for one simulation.

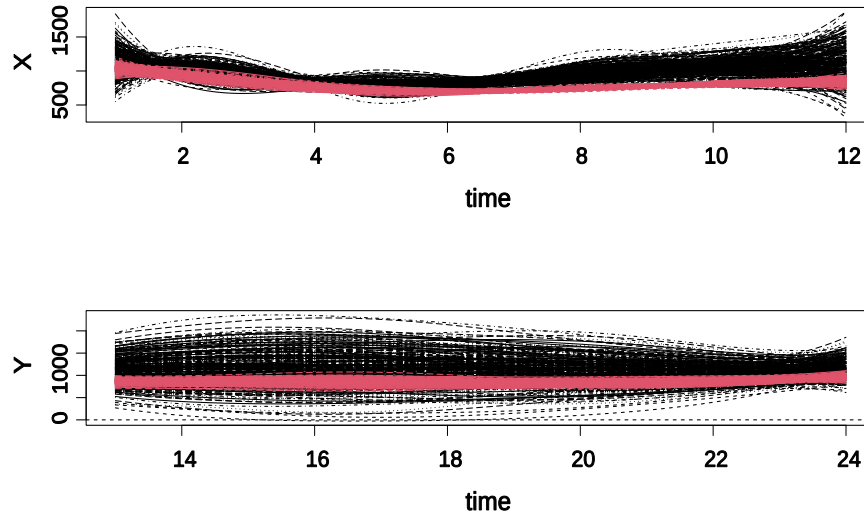


Fig. 3 Smooth data simulated according to scenario 2 colored by group for one simulation.

good results. For the more difficult clustering problem in scenario 2, taking into account the relationship between Y_i and X_i seems to matter and only `funWeightClust` succeeds to find the correct partition.

Table 3 Mean (and standard deviation) of ARI for BIC best model on 100 simulations. Bold values indicate the highest value for each method.

Scenario	Method	ϵ	ARI
1	FunHDDC	0.005	0.8589641 (0.1401613)
1	FunHDDC	0.01	0.8527159(0.1375641)
1	FunHDDC	0.2	0.7264915 (0.1236281)
1	2D-funHDDC	0.005	0.2791434 (0.04373348)
1	2D-funHDDC	0.01	0.2791434(0.04373348)
1	2D-funHDDC	0.2	0.270681 (0.05636388)
1	funWeightClust	0.005	0.9965396 (0.006011004)
1	funWeightClust	0.01	0.9960756(0.006813709)
1	funWeightClust	0.2	0.1535521 (0.0371209)
2	FunHDDC	0.005	0.1309167 (0.04842073)
2	FunHDDC	0.01	0.1309442(0.04844203)
2	FunHDDC	0.2	0.1220269 (0.04650234)
2	2D-funHDDC	0.005	0.1256394 (0.02688633)
2	2D-funHDDC	0.01	0.1256394(0.02688633)
2	2D-funHDDC	0.2	0.1462503 (0.04981952)
2	funWeightClust	0.005	0.8333807 (0.1946126)
2	funWeightClust	0.01	0.8380116(0.1856003)
2	funWeightClust	0.2	0.06956302(0.0255526)

5.2 Benchmark study- Adelaide electricity demand data

The Adelaide data is available in the *fds* package in R and consist of electricity demands, in Megawatt (MW) from Sunday to Saturday in Adelaide, Australia for 508 weeks, between July 6, 1976 and March 31, 2007 (Magnano et al, 2008). The electricity demand is measured half-hourly, i.e. we have 48 time points in a day, and we have 508×7 daily curves. These data were used to fit concurrent functional regression models (Ramsay and Silverman, 2006) and non-linear function-on-function regression models using neural networks for the dependency of electricity demand on temperature (Rao and Reimherr, 2021).

We restrict our analysis to Sundays and Tuesdays, so we have 1016 daily curves (see Figure 4). We suppose that the electricity demand in the morning can be used to predict the demand in the afternoon, so the covariate X_i includes the first 24 points (from midnight to noon) and the last 24 points (from noon to midnight) are measurements corresponding to the response Y_i . Electricity demand follows different dynamics on weekends (Sunday) compared to weekdays (Tuesday), so we apply funWeightClust to partition into these two groups.

For comparison we also apply funHDDC to the combined curves and 2D-funHDDC, where, as before, by 2D-funHDDC we denote funHDDC applied to the two-dimensional curves (X_i, Y_i) . Curves are smoothed using cubic B-splines with 6 basis elements. We run the algorithms for $K = 2$ clusters using $\epsilon \in \{0.01, 0.1, 0.2\}$ in the Cattell test, and the best solution in terms of the highest BIC value for all sub-models is returned. The initialization is done using *kmeans* method with 20 repetitions, and the maximum number of iterations is 200.

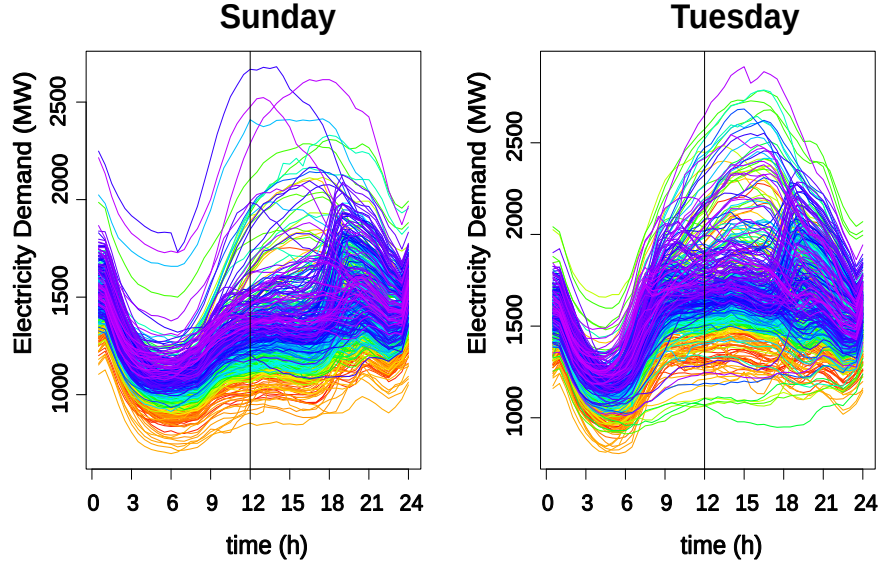


Fig. 4 Electricity demand in Adelaide for Sundays and Tuesdays, between July 6, 1976 and March 31, 2007

We compare funWeightClust also with *kmeans* (from the R *stats* package), flexmix (from the R package *flexmix*), and Mclust (from the *mclust* R package), applied to the raw data and also applied as two-steps methods to the coefficients of the cubic B-spline basis with 6 basis elements. For flexmix we consider the data corresponding to the pairs (X_i, Y_i) , and for the other methods we work with the data corresponding to the combined curves defined on the whole interval $[0, 24]$.

Table 4 ARI for each method for the Adelaide data

Method	ϵ	ARI	Method	ϵ	ARI	Method	ARI
funHDDC	0.01	0.48	2D-funHDDC	0.2	0.53	<i>kmeans</i> -two-steps method	0.55
funHDDC	0.1	0.50	funWeightClust	0.01	0.61	flexmix-raw data	-0.000
funHDDC	0.2	0.48	funWeightClust	0.1	0.94	flexmix-two-steps method	-0.000
2D-funHDDC	0.01	0.34	funWeightClust	0.2	0.85	Mclust-raw data	0.002
2D-funHDDC	0.1	0.47	<i>kmeans</i> -raw data	-	0.48	Mclust-two-steps method	0.001

The results in Table 4 clearly show that funWeightClust outperforms the other methods, and for $\epsilon = 0.1$ we obtain ARI=0.94, so a very accurate clustering. The clusters obtained with funWeightClust with $\epsilon = 0.1$ are presented in Figure 5.

From the results in Table 4 it seems that the difference between the electricity demand on Sundays and Tuesday is illustrated the best by the different relationship between the electricity demand in the mornings (X_i) and in the afternoons (Y_i). The only methods that consider the dependency between Y_i and X_i are flexmix and

funWeightClust, but flexmix does not account for correlated multivariate response variables and gives poor results for both the raw data and the data represented by the coefficients of the cubic B-splines. funHDDC and *kmeans* give the second best results, but these methods cluster the curves defined on the whole interval $[0, 24]$.

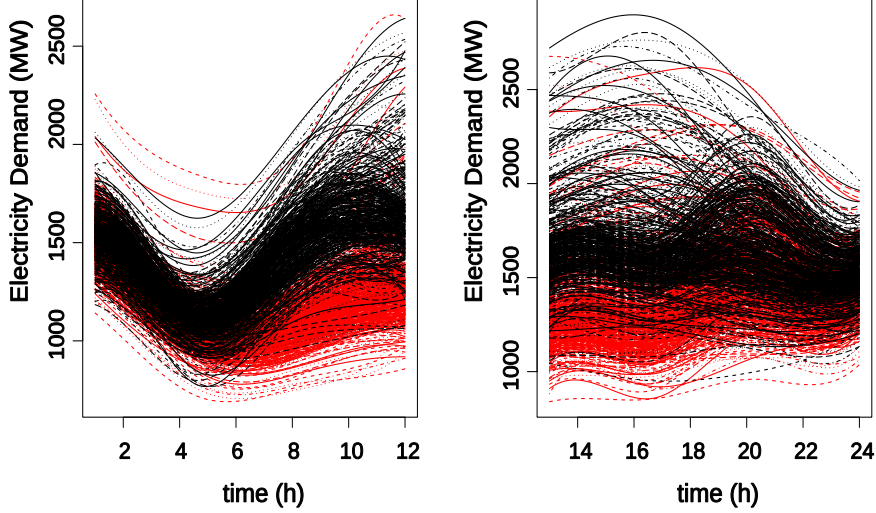


Fig. 5 Clustering with funWeightClust ($\epsilon = 0.1$) of electricity demand in Adelaide for Sundays (red) and Tuesdays (black)

5.3 Real data example- Traffic Speeding

We use funWeightClust on speeding differential data extracted from speed surveys conducted by the City of Edmonton during the summer months of 2017 and 2018 available from an open data portal (<https://data.edmonton.ca/stories/s/Speed-Surveys/kd7n-5iq3/>). We expect patterns to appear between the prediction of afternoon traffic (8:15 am – 11:45 pm) from the morning traffic rush (12 am – 8 am). Traffic data for car going 5 – 10 km/h under the speed limit (bin 2) and 0 – 5 km/h over the speed limit (bin 4) are considered. The X_i part of the regression consists of the bin 2 and bin 4 morning traffic data, and the Y_i component is the afternoon traffic, making this a multivariate traffic functional regression clustering problem. Data are composed of car counts recorded every 15 minutes. The observations are recorded for each X_i bi-dimensional curve at 36 time points (12 am – 8 am) and for each Y_i bi-dimensional curve at the remaining 60 time points (8:15 am – 11:45 pm).

A thousand records are sampled from the original data set for clustering with the funWeightClust method. We take the best result using the BIC criterion and compare the clustered curves by their locations in the city and speed limits. The objective of

this study is to find patterns of traffic regressions related to travel preferences on roads. These results are the first step of an in-depth analysis of how morning and evening traffic affect each other and the trends that appear in this relationship.

Data are fit with a B-Spline basis using 6 basis functions for each component of the X_i and Y_i functional data. We use all models of the funWeightClust method, considering a range of clusters from 2 to 10. The best result was 4 clusters and a threshold for the Cattell test $\epsilon = 0.001$.

The funWeightClust method clusters the data according to the different ways the traffic in the morning rush predicts the afternoon traffic. Within the four clusters, shown in Figure 6, we discern two large clusters (1 and 2) and two smaller clusters (3 and 4). Each cluster has distinct patterns of behavior of peaking only in the evening or peaking in the evening and morning. Clusters 3 and 4 have low amounts of travel, creating different patterns of behavior than clusters 1 and 2 in the response variable. From table 5 we see that while most of the data is recorded on roads with maximum speed limits of 50 and 60 km/h, the data for groups 3 and 4 are recorded mostly on roads with maximum speed limits of 50 and 30 km/h. Using latitude and longitude we identified that roads from clusters 3 and 4 are close to main roads networks. These roads may be neighborhood roads or side roads used as detours during rush hour.

Table 5 Maximum speed limit for the roads where the measurements were done for each cluster

Maximum speed limit	cluster 1	cluster 2	cluster 3	cluster 4
30	37	0	14	10
40	6	0	0	0
50	230	66	84	51
60	252	226	4	7
70	4	9	0	0

6 Conclusions and future work

We propose the method funWeightClust for clustering heterogeneous functional linear regression data. Based on a cluster weighted model for functional data and on a multivariate functional principal component analysis, funWeightClust has the important advantage that it can handle functional multivariate responses and predictors. We include the distribution of the coefficients of the covariates in the likelihood, and we construct an EM algorithm to estimate the parameters. Despite the complexity of the model, the maximization of the complete log likelihood can be done in closed form expressions. To add model flexibility, we consider several two-component parsimonious models by combining the parsimonious models used for funHDDC (Bouveyron and Jacques, 2011) with the Gaussian parsimonious clustering models family in Celeux and Govaert (1995).

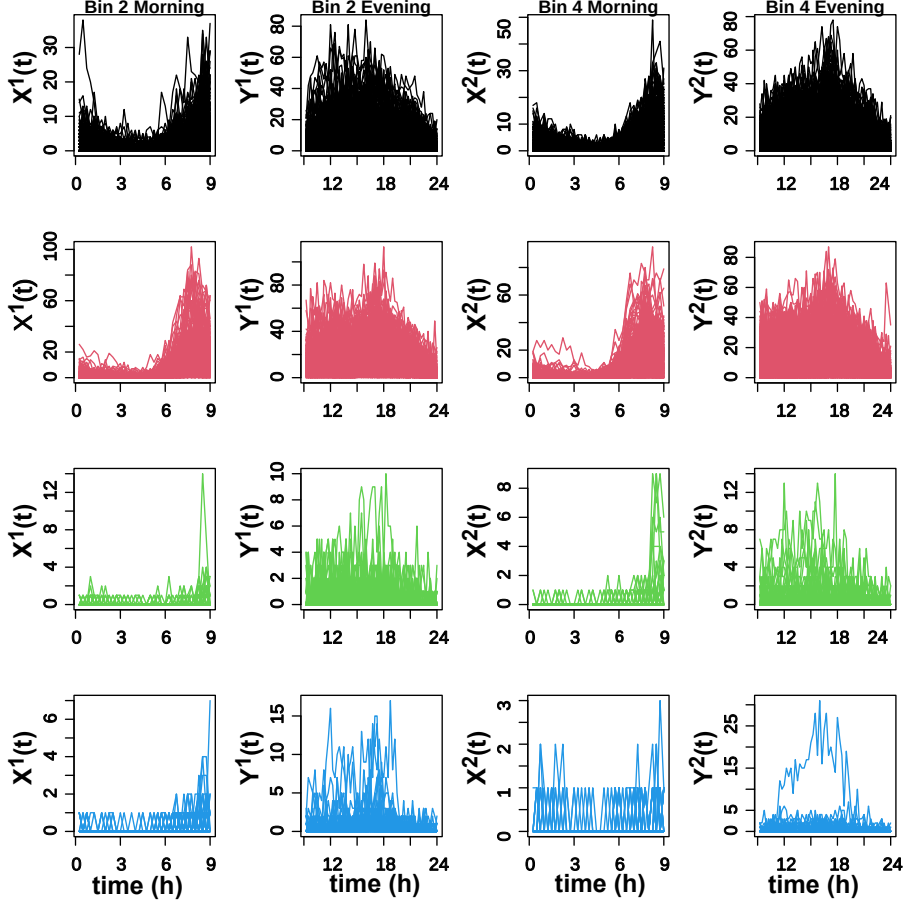


Fig. 6 Clustering with funWeightClust of Edmonton's traffic data

We conduct experiments for simulated data and for the Adelaide electricity demand data in the *fds* R package, and compare the proposed method funWeightClust with funHDDC and two-steps methods based on clustering methods for multivariate data. For simulated data that include linear regression dependencies between the variables, funWeightClust outperforms funHDDC. The differences between the Adelaide electricity demand during Sundays and Tuesday are captured very precisely by funWeightClust, with an ARI=0.94, much larger than the results obtained using the other methods.

We also use funWeightClust to cluster speeding data in Edmonton, Alberta. The proposed clusterwise functional regression model captures the dependence of the afternoon traffic on the morning traffic. Using funWeightClust we were able to identify groups that show how the roads are utilized during the morning and afternoon rush hours. For cities like Edmonton, the analysis of traffic flow is crucial in transportation planning and optimization of road design.

The proposed model is based on multivariate Gaussian distributions. Our approach can be extended to non-Gaussian mixture models by considering multivariate skewed

distributions as in [Gallaugher et al \(2022\)](#). Here we focus on unsupervised learning, but a similar methodology can be applied for functional classification and prediction ([Chiou et al, 2016](#), [Chiou, 2012](#)).

Appendix A Proof of Proposition 2

Proof. The complete-data likelihood can be written as the product of the conditional densities of the multivariate response $\mathbf{c}_{Y,i}$ given the covariates $\mathbf{c}_{X,i}$ and $\mathbf{Z}_i = \mathbf{z}_i$, the conditional densities of $\mathbf{c}_{X,i}$ given that $\mathbf{Z}_i = \mathbf{z}_i$, and the marginal densities of the $\mathbf{Z}_i$:

$$L_c(\boldsymbol{\theta}) = \prod_{i=1}^n \prod_{k=1}^K \left\{ \phi(\mathbf{c}_{Y,i}; \boldsymbol{\mu}_{Y,k}, \boldsymbol{\Sigma}_{Y,k}) \phi(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k}) \pi_k \right\}^{z_{ik}},$$

where $z_{ik} = 1$ if $(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i})$ belongs to the cluster k and $z_{ik} = 0$ otherwise. Thus, the complete-data log-likelihood can be written as

$$l_c(\boldsymbol{\theta}) = l_{1c}(\pi) + l_{2c}(\boldsymbol{\vartheta}_X) + l_{3c}(\boldsymbol{\vartheta}_Y)$$

where

$$\begin{aligned} l_{1c}(\pi) &= \sum_{i=1}^n \sum_{k=1}^K z_{ik} \log(\pi_k) \\ l_{2c}(\boldsymbol{\vartheta}_X) &= -\frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K z_{ik} \left(R_X \log(2\pi) + \log |\boldsymbol{\Sigma}_{X,k}| + (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) \right) \end{aligned} \quad (\text{A1})$$

$$\begin{aligned} l_{3c}(\boldsymbol{\vartheta}_Y) &= -\frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K z_{ik} \left(R_Y \log(2\pi) + \log |\boldsymbol{\Sigma}_{Y,k}| + (\mathbf{c}_{Y,i} - \boldsymbol{\mu}_{Y,k})^\top \boldsymbol{\Sigma}_{Y,k}^{-1} (\mathbf{c}_{Y,i} - \boldsymbol{\mu}_{Y,k}) \right) \\ &= -\frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K z_{ik} \left(R_Y \log(2\pi) + \log |\boldsymbol{\Sigma}_{Y,k}| + (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \right. \\ &\quad \left. (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*) \right) \end{aligned} \quad (\text{A2})$$

From (16) we have

$$\boldsymbol{\Sigma}_{X,k}^{-1} = \mathbf{W}_X^{1/2} \mathbf{Q}_k \mathbf{D}_k^{-1} \mathbf{Q}_k^\top \mathbf{W}_X^{1/2},$$

and

$$|\boldsymbol{\Sigma}_{X,k}| = |\mathbf{D}_k| |\mathbf{W}_X|^{-1} |\mathbf{Q}_k^\top \mathbf{Q}_k| = |\mathbf{D}_k| |\mathbf{W}_X|^{-1} = |\mathbf{W}_X|^{-1} \prod_{l=1}^{d_k} a_{kl} \prod_{l=d_k+1}^{R_X} b_k. \quad (\text{A3})$$

Moreover, since $(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})$ is a scalar, we get

$$\begin{aligned} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) &= \text{trace}((\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{Q}_k \mathbf{D}_k^{-1} \mathbf{Q}_k^\top \mathbf{W}_X^{1/2} \\ (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) &= \text{trace}\left(\left((\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{Q}_k\right) \left(\mathbf{D}_k^{-1} \mathbf{Q}_k^\top \mathbf{W}_X^{1/2} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})\right)\right) \\ &= \text{trace}\left(\left(\mathbf{D}_k^{-1} \mathbf{Q}_k^\top \mathbf{W}_X^{1/2} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})\right) \left((\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{Q}_k\right)\right) \end{aligned} \quad (\text{A4})$$

Replacing in (A1) we obtain

$$\begin{aligned} l_{2c}(\boldsymbol{\vartheta}_X) &= -\frac{nR_X \log(2\pi)}{2} + \frac{n}{2} \log(|\mathbf{W}_X|) - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=1}^{d_k} \log(a_{kl}) - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=d_k+1}^{R_X} \log(b_k) \\ &\quad - \frac{1}{2} \sum_{k=1}^K \text{trace}\left(\left(\mathbf{D}_k^{-1} \mathbf{Q}_k^\top \mathbf{W}_X^{1/2}\right) \left(\sum_{i=1}^n z_{ik} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top\right) \left(\mathbf{W}_X^{1/2} \mathbf{Q}_k\right)\right). \end{aligned}$$

We can rewrite $l_{2c}(\boldsymbol{\vartheta}_X)$ as

$$\begin{aligned} l_{2c}(\boldsymbol{\vartheta}_X) &= -\frac{nR_X \log(2\pi)}{2} + \frac{n}{2} \log(|\mathbf{W}_X|) - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=1}^{d_k} \log(a_{kl}) \\ &\quad - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=d_k+1}^{R_X} \log(b_k) - \frac{1}{2} \sum_{k=1}^K \text{trace}\left(\mathbf{D}_k^{-1} \mathbf{Q}_k^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k} \mathbf{W}_X^{1/2} \mathbf{Q}_k\right) \\ &= -\frac{nR_X \log(2\pi)}{2} + \frac{n}{2} \log(|\mathbf{W}_X|) - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=1}^{d_k} \log(a_{kl}) - \frac{1}{2} \sum_{k=1}^K n_k \sum_{l=d_k+1}^{R_X} \log(b_k) \\ &\quad - \frac{1}{2} \sum_{k=1}^K \left(\sum_{l=1}^{d_k} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{a_{kl}} + \sum_{l=d_k+1}^{R_X} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{b_k} \right), \end{aligned}$$

where $\mathbf{q}_{kl}$ is the l th column of $\mathbf{Q}_k$, $\mathbf{S}_{X,k}$ is defined in (24), and $\boldsymbol{\vartheta}_X = \{\boldsymbol{\mu}_{X,k}, a_{kj}, b_k, \mathbf{q}_{kj}\}$, $k = 1, \dots, K$, $j = 1, \dots, d_k$.

Next, from (A2) we have

$$\begin{aligned} l_{3c}(\boldsymbol{\vartheta}_Y) &= -\frac{nR_Y \log(2\pi)}{2} - \frac{1}{2} \sum_{k=1}^K n_k \log(\log |\boldsymbol{\Sigma}_{Y,k}|) - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K z_{ik} \left(\mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} \right. \\ &\quad \left. - \mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* - (\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} + (\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* \right) \end{aligned}$$

□

Appendix B Proof of Proposition 3

Proof. From (A4) we obtain

$$(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) \quad (\text{B5})$$

$$\begin{aligned} &= \left(\sum_{l=1}^{d_k} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{a_{kl}} \right. \\ &\quad \left. + \sum_{l=d_k+1}^R \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{b_k} \right) \\ &= \delta(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \mathbf{Q}_k, a, b, d_k). \end{aligned} \quad (\text{B6})$$

Replacing in (19) and using also (14), (17), and (A3) we obtain

$$\begin{aligned} p_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k) &= \phi(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \boldsymbol{\Sigma}_{X,k}) \phi(\mathbf{c}_{Y,i}; \boldsymbol{\mu}_{Y,k}, \boldsymbol{\Sigma}_{Y,k}) \\ &= (2\pi)^{-(R_X+R_Y)/2} |\boldsymbol{\Sigma}_{X,k}|^{-1/2} |\boldsymbol{\Sigma}_{Y,k}|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1} \right. \\ &\quad \left. (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) - \frac{1}{2}(\mathbf{c}_{Y,i} - \boldsymbol{\mu}_{Y,k})^\top \boldsymbol{\Sigma}_{Y,k}^{-1} (\mathbf{c}_{Y,i} - \boldsymbol{\mu}_{Y,k})\right) \\ &= (2\pi)^{-(R_X+R_Y)/2} \left(\prod_{j=1}^{d_k} a_{kj} \prod_{j=d_k+1}^{R_X} b_k \right)^{-1/2} |\mathbf{W}_X|^{1/2} |\boldsymbol{\Sigma}_{Y,k}|^{-1/2} \\ &\quad \exp\left(-\frac{1}{2}\delta(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \mathbf{Q}_k, a, b, d_k) - \frac{1}{2}(\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \right. \\ &\quad \left. (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)\right) \\ &= (2\pi)^{-(R_X+R_Y)/2} |\mathbf{W}_X|^{1/2} \exp\left(-\frac{1}{2}\left(\sum_{j=1}^{d_k} \log(a_{kj}) + (R_X - d_k) \log(b_k) \right. \right. \\ &\quad \left. \left. + \log(|\boldsymbol{\Sigma}_{Y,k}|) + \delta(\mathbf{c}_{X,i}; \boldsymbol{\mu}_{X,k}, \mathbf{Q}_k, a, b, d_k) + (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \right. \right. \\ &\quad \left. \left. (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)\right)\right) \\ &= (2\pi)^{-(R_X+R_Y)/2} |\mathbf{W}_X|^{1/2} \pi_k^{-1} \exp\left(-\frac{1}{2}H_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k)\right), \end{aligned}$$

where $H_k(\mathbf{c}_{Y,i}, \mathbf{c}_{X,i} \mid \boldsymbol{\theta}_k)$ is defined in (25). $\square$

Appendix C Proof of Proposition 4

Proof. Using (20)-(23) we have that $Q(\boldsymbol{\theta} \mid \boldsymbol{\theta}^{(m-1)})$ is given by

$$Q(\boldsymbol{\theta} \mid \boldsymbol{\theta}^{(m-1)}) = Q_1(\pi \mid \boldsymbol{\theta}^{(m-1)}) + Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) + Q_3(\boldsymbol{\vartheta}_Y \mid \boldsymbol{\theta}^{(m-1)}),$$

were

$$\begin{aligned} Q_1(\pi \mid \boldsymbol{\theta}^{(m-1)}) &= \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} \log(\pi_k) \\ Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) &= -\frac{nR_X \log(2\pi)}{2} + \frac{n}{2} \log(|\mathbf{W}_X|) \\ &\quad - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \sum_{l=1}^{d_k} \log(a_{kl}) - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \sum_{l=d_k+1}^{R_X} \log(b_k) \\ &\quad - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \left(\sum_{l=1}^{d_k} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{a_{kl}} + \sum_{l=d_k+1}^{R_X} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{b_k} \right), \\ Q_3(\boldsymbol{\vartheta}_Y \mid \boldsymbol{\theta}^{(m-1)}) &= -\frac{nR_Y \log(2\pi)}{2} - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log(|\boldsymbol{\Sigma}_{Y,k}|) \\ &\quad - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} (\mathbf{c}_{Y,i} - \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^*) \end{aligned}$$

where $\mathbf{S}_{X,k}^{(m)}$ is defined in (28).

For the estimation of $\pi_k, k = 1, \dots, K$ we introduce the Lagrange multiplier λ and we maximize $Q_1 = Q_1(\pi \mid \boldsymbol{\theta}^{(m-1)}) - \lambda(\sum_{k=1}^K \pi_k - 1)$. We get (29) solving the system

$$\frac{\partial Q_1}{\partial \pi_k} = \sum_{i=1}^n \frac{t_{ik}^{(m)}}{\pi_k} - \lambda = 0, k = 1, \dots, K \quad \frac{\partial Q_1}{\partial \lambda} = \sum_{k=1}^K \pi_k - 1 = 0.$$

To get an update for $\boldsymbol{\mu}_{X,k}^{(m)}$ we calculate $Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)})$ starting from the formula (A1) and we obtain

$$\begin{aligned} Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) &= -\frac{n}{2} R_X \log(2\pi) - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log |\boldsymbol{\Sigma}_{X,k}| \\ &\quad - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k})^\top \boldsymbol{\Sigma}_{X,k}^{-1} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}). \end{aligned}$$

The gradient of Q_2 with respect to $\boldsymbol{\mu}_{X,k}$ is

$$\begin{aligned}\nabla_{\boldsymbol{\mu}_{X,k}} Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) &= -\sum_{i=1}^n t_{ik}^{(m)} \boldsymbol{\Sigma}_{X,k}^{-1} (\mathbf{c}_{X,i} - \boldsymbol{\mu}_{X,k}) \\ &= \boldsymbol{\Sigma}_{X,k}^{-1} \left(-\sum_{i=1}^n t_{ik}^{(m)} \mathbf{c}_{X,i} + \boldsymbol{\mu}_{X,k} \sum_{i=1}^n t_{ik}^{(m)} \right).\end{aligned}$$

Thus, we can easily get (30) solving $\nabla_{\boldsymbol{\mu}_{X,k}} Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) = \mathbf{0}$.

To estimate $\mathbf{Q}_k$ we have to maximize $Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)})$ with respect to $\mathbf{q}_{kl}$ under the constraint $\mathbf{q}_{kl}^\top \mathbf{q}_{kl} = 1$. This is equivalent with minimizing $-2Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)})$ with respect to $\mathbf{q}_{kl}$ under this constraint, so we consider the function $Q_{2c} = -2Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) - \sum_{l=1}^{R_X} \omega_{kl} (\mathbf{q}_{kl}^\top \mathbf{q}_{kl} - 1)$, where ω_{kl} are Lagrange multipliers. The gradient of Q_{2c} with respect to $\mathbf{q}_{kl}$ is

$$\begin{aligned}\nabla_{\mathbf{q}_{kl}} Q_{2c} &= 2n_k^{(m)} \frac{\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{\Sigma_{kl}} - 2\omega_{kl} \mathbf{q}_{kl}, \\ \Sigma_{kl} &= \begin{cases} a_{kl} & \text{if } l = 1, \dots, d_k \\ b_k & \text{if } l = d_k + 1, \dots, R_X. \end{cases}\end{aligned}$$

From $\nabla_{\mathbf{q}_{kl}} Q_{2c} = 0$ we get $\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl} = \frac{\omega_{kl} \Sigma_{kl}}{n_k^{(m)}} \mathbf{q}_{kl}$, so $\mathbf{q}_{kl}$ is an eigenfunction of $\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}$ and the associated eigenvalue is $\lambda_{kl}^{(m)} = \frac{\omega_{kl} \Sigma_{kl}}{n_k^{(m)}}$. Notice that we also have $\mathbf{q}_{kl}^\top \mathbf{q}_{kj} = 0$ if $l \neq j$, and $\lambda_{kl}^{(m)} = \mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}$ so we can write

$$\begin{aligned}-2Q_2(\boldsymbol{\vartheta}_X \mid \boldsymbol{\theta}^{(m-1)}) &= nR_X \log(2\pi) - n \log(|\mathbf{W}_X|) + \sum_{k=1}^K n_k^{(m)} \left(\sum_{l=1}^{d_k} \log(a_{kl}) \right. \\ &\quad \left. + \sum_{l=d_k+1}^{R_X} \log(b_k) \right) + \sum_{k=1}^K n_k^{(m)} \left(\sum_{l=1}^{d_k} \frac{\lambda_{kl}^{(m)}}{a_{kl}} + \sum_{l=d_k+1}^{R_X} \frac{\lambda_{kl}^{(m)}}{b_k} \right) \\ &= nR_X \log(2\pi) - n \log(|\mathbf{W}_X|) + \sum_{k=1}^K n_k^{(m)} \left(\sum_{l=1}^{d_k} \log(a_{kl}) + \sum_{l=d_k+1}^{R_X} \log(b_k) \right) \\ &\quad + \sum_{k=1}^K n_k^{(m)} \left(\sum_{l=1}^{d_k} \lambda_{kl}^{(m)} \left(\frac{1}{a_{kl}} - \frac{1}{b_k} \right) + \frac{1}{b_k} \text{trace}(\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}) \right).\end{aligned}$$

Here we have also used

$$\text{trace}(\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}) = \sum_{l=1}^{R_X} \lambda_{kl}^{(m)} = \sum_{l=1}^{d_k} \lambda_{kl}^{(m)} + \sum_{l=d_k+1}^{R_X} \lambda_{kl}^{(m)}. \quad (\text{C7})$$

Since for any $l = 1, \dots, d_k$ we have $a_{kl} \geq b_k$, we get $\frac{1}{a_{kl}} - \frac{1}{b_k} \leq 0$, so $\sum_{l=1}^{d_k} \lambda_{kl}^{(m)} \left(\frac{1}{a_{kl}} - \frac{1}{b_k} \right)$ is a decreasing function of λ_{kl} . Thus, we estimate $\mathbf{q}_{kl}$ by the eigenfunction associated with the l th highest eigenvalue of $\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}$.

To update a_{kl} we solve

$$\frac{\partial Q_2(\boldsymbol{\vartheta}_X | \boldsymbol{\theta}^{(m-1)})}{\partial a_{kl}} = -\frac{n_k^{(m)}}{2a_{kl}} + \frac{n_k^{(m)} \mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{2a_{kl}^2} = 0,$$

and we get $a_{kl}^{(m)} = \mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl} = \lambda_{kl}^{(m)}$, the l th highest eigenvalue of $\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}$.

From

$$\frac{\partial Q_2(\boldsymbol{\vartheta}_X | \boldsymbol{\theta}^{(m-1)})}{\partial b_k} = -\frac{n_k^{(m)}}{2} \sum_{l=d_k+1}^{R_X} \frac{1}{b_k} + \frac{n_k^{(m)}}{2} \sum_{l=d_k+1}^{R_X} \frac{\mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl}}{b_k^2} = 0,$$

we obtain

$$b_k^{(m)} = \frac{1}{R_X - d_k} \sum_{l=d_k+1}^{R_X} \mathbf{q}_{kl}^\top \mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2} \mathbf{q}_{kl} = \frac{1}{R_X - d_k} \sum_{l=d_k+1}^{R_X} \lambda_{kl}^{(m)}$$

Thus, using (C7) we get

$$b_k^{(m)} = \frac{1}{R_X - d_k} \left(\text{trace}(\mathbf{W}_X^{1/2} \mathbf{S}_{X,k}^{(m)} \mathbf{W}_X^{1/2}) - \sum_{l=1}^{d_k} \lambda_{kl}^{(m)} \right).$$

To estimate the regression coefficient we use the properties of trace and transpose and $\boldsymbol{\Sigma}_{Y,k}^\top = \boldsymbol{\Sigma}_{Y,k}$ and we get

$$\begin{aligned} Q_3(\boldsymbol{\vartheta}_Y | \boldsymbol{\theta}^{(m-1)}) &= -\frac{nR_y \log(2\pi)}{2} - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log(|\boldsymbol{\Sigma}_{Y,k}|) \\ &\quad - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} \left(\mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} - \text{trace} \left(\mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* \right) \right. \\ &\quad \left. - \text{trace} \left((\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} \right) + \text{trace} \left((\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* \right) \right) \\ &= -\frac{nR_y \log(2\pi)}{2} - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log(|\boldsymbol{\Sigma}_{Y,k}|) - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} \left(\mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} \right. \\ &\quad \left. - \text{trace} \left(\boldsymbol{\Gamma}_*^k \mathbf{c}_{X,i}^* \mathbf{c}_{Y,i}^\top \boldsymbol{\Sigma}_{Y,k}^{-1} \right) - \text{trace} \left(\boldsymbol{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} (\mathbf{c}_{X,i}^*)^\top (\boldsymbol{\Gamma}_*^k)^\top \right) \right) \end{aligned}$$

$$\begin{aligned}
& + \text{trace} \left(\mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^* (\mathbf{c}_{X,i}^*)^\top \left(\mathbf{\Gamma}_*^k \right)^\top \mathbf{\Sigma}_{Y,k}^{-1} \right) \\
& = -\frac{nR_y \log(2\pi)}{2} - \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log(|\mathbf{\Sigma}_{Y,k}|) - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} \left(\mathbf{c}_{Y,i}^\top \mathbf{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} \right. \\
& \quad \left. - 2 \text{trace} \left(\mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^* \mathbf{c}_{Y,i}^\top \mathbf{\Sigma}_{Y,k}^{-1} \right) + \text{trace} \left(\mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^* (\mathbf{c}_{X,i}^*)^\top \left(\mathbf{\Gamma}_*^k \right)^\top \mathbf{\Sigma}_{Y,k}^{-1} \right) \right)
\end{aligned}$$

To update $\mathbf{\Gamma}_*^k$ we solve

$$\frac{\partial Q_3(\boldsymbol{\vartheta}_Y \mid \boldsymbol{\theta}^{(m-1)})}{\partial \mathbf{\Gamma}_*^k} = \mathbf{0}, \quad (\text{C8})$$

$$-\frac{1}{2} \sum_{i=1}^n t_{ik}^{(m)} \left(-2 \mathbf{\Sigma}_{Y,k}^{-1} \mathbf{c}_{Y,i} (\mathbf{c}_{X,i}^*)^\top + 2 \mathbf{\Sigma}_{Y,k}^{-1} \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^* (\mathbf{c}_{X,i}^*)^\top \right) = \mathbf{0}. \quad (\text{C9})$$

Thus for any $k = 1, \dots, K$ we obtain

$$(\mathbf{\Gamma}_*^k)^{(m)} = \left(\sum_{i=1}^n t_{ik}^{(m)} \mathbf{c}_{Y,i} (\mathbf{c}_{X,i}^*)^\top \right) \left(\sum_{i=1}^n t_{ik}^{(m)} \mathbf{c}_{X,i}^* (\mathbf{c}_{X,i}^*)^\top \right)^{-1}.$$

Notice that using again properties of trace and transpose we have

$$\begin{aligned}
Q_3(\boldsymbol{\vartheta}_Y \mid \boldsymbol{\theta}^{(m-1)}) & = -\frac{nR_y \log(2\pi)}{2} + \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log(|\mathbf{\Sigma}_{Y,k}^{-1}|) \\
& \quad - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} \text{trace} \left((\mathbf{c}_{Y,i} - \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \mathbf{\Sigma}_{Y,k}^{-1} (\mathbf{c}_{Y,i} - \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^*) \right) \\
& = -\frac{nR_y \log(2\pi)}{2} + \frac{1}{2} \sum_{k=1}^K n_k^{(m)} \log(|\mathbf{\Sigma}_{Y,k}^{-1}|) \\
& \quad - \frac{1}{2} \sum_{i=1}^n \sum_{k=1}^K t_{ik}^{(m)} \text{trace} \left(\mathbf{\Sigma}_{Y,k}^{-1} (\mathbf{c}_{Y,i} - \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^*) (\mathbf{c}_{Y,i} - \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top \right)
\end{aligned}$$

Taking the derivative we obtain

$$\begin{aligned}
& \frac{\partial Q_3(\boldsymbol{\vartheta}_Y \mid \boldsymbol{\theta}^{(m-1)})}{\partial \mathbf{\Sigma}_{Y,k}^{-1}} = \mathbf{0}, \\
& \frac{1}{2} n_k^{(m)} \left(\mathbf{\Sigma}_{Y,k}^{-1} \right)^{-1} - \frac{1}{2} \sum_{i=1}^n t_{ik}^{(m)} (\mathbf{c}_{Y,i} - \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^*) (\mathbf{c}_{Y,i} - \mathbf{\Gamma}_*^k \mathbf{c}_{X,i}^*)^\top = \mathbf{0}.
\end{aligned}$$

Thus

$$\Sigma_{Y,k}^{(m)} = \frac{\sum_{i=1}^n t_{ik}^{(m)} (\mathbf{c}_{Y,i} - (\mathbf{\Gamma}_*^k)^{(m)} \mathbf{c}_{X,i}^*) (\mathbf{c}_{Y,i} - (\mathbf{\Gamma}_*^k)^{(m)} \mathbf{c}_{X,i}^*)^\top}{n_k^{(m)}}$$

□

Appendix D Regression coefficients for simulations in Section 5.1

$$\mathbf{\Gamma}_0^1 = (40.55785, -136.39392, 364.48536, -1009.44904, 137.08185, -53.19644)^\top, \mathbf{\Gamma}_0^2 = (10.55038, -94.09524, 386.14923, -886.60180, 105.71551, 250.83997)^\top,$$

$$\mathbf{\Gamma}^1 = \begin{pmatrix} 0.1604788 & -0.006105744 & -0.34002176 & 0.8045786 & -1.809933 & 3.1085371 \\ 0.0216076 & 0.360282816 & 0.02519028 & 0.0829196 & -1.394305 & 2.9290406 \\ -1.5683676 & 1.279807057 & -2.81184706 & 4.6599002 & -6.812895 & 7.9705907 \\ 3.2542660 & -0.769508698 & 1.18667337 & -2.3600145 & 2.725763 & -1.9297317 \\ -2.1495590 & 2.106397045 & -0.45220970 & -0.5759578 & 1.517537 & -0.9133536 \\ 1.8634967 & -1.706644614 & 1.91048360 & -1.6978476 & 1.125397 & -0.1015894 \end{pmatrix},$$

$$\mathbf{\Gamma}^2 = \begin{pmatrix} -0.3061923 & 0.59565429 & -0.8955555 & 1.1888545 & -1.8901795 & 3.07764911 \\ -0.2590663 & 1.36715364 & -2.1170851 & 2.4453460 & -3.2342896 & 4.11607039 \\ -1.2827794 & 0.52439869 & -0.9992164 & 2.1114220 & -4.0969844 & 5.91743174 \\ 4.5782789 & -0.04588379 & -1.9809570 & 0.6746645 & -0.2431451 & 1.01274374 \\ 0.8890119 & 0.15656989 & -0.6024806 & 0.4886304 & -0.6317594 & 1.18570678 \\ 2.8875206 & -1.88979145 & 0.9503891 & -0.8400636 & 0.6522031 & -0.02998784 \end{pmatrix}.$$

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Code availability. The R Code used for the numerical experiments is available upon request.

Declarations

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