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Abstract: We consider the variable selection problem in multivariate linear models where the predictors are given as functions and the responses are scalars, with the help of sparse regularization. Observations corresponding to the predictors are supposed to be measured repeatedly at discrete time points, and then they are treated as smooth functional data. Parameters included in the functional multivariate linear model are estimated by the penalized least squared method with the ℓ_1/ℓ_2 type penalty. We construct a blockwise coordinate descent algorithm for deriving the estimates of the functional multivariate linear model. A tuning parameter which control the degree of the regularization is decided by information criteria. In order to investigate the effectiveness of the proposed method we apply it to the analysis of simulated data and real data.

Key Words and Phrases: Lasso, Multivariate regression model, Functional data analysis, Regularization, Variable selection

1 Introduction

Functional data analysis (FDA) has received considerable attention in different fields of application, including bioscience, system engineering, and meteorology, and a number of applications have been reported (see, e.g., Ramsay and Silverman, 2005; Horváth and Kokoszka, 2012). The basic idea behind functional data analysis is to express data observed longitudinally as a smooth function and then draw information from the collection of functional data.

Functional regression analysis that models the relationship between predictors and responses given as functions have been widely studied. Many of the works are assigned to models with functional predictors and scalar responses (James, 2002; Cardot et al., 2003; Rossi et al., 2005; Müller and Yao, 2008, and references therein), on the other hand, models with functional predictors and functional responses are also considered in Malfait and Ramsay (2003), Yao et al. (2005), Harezlak et al. (2007) and Matsui et al. (2009). In this paper we consider constructing the functional regression model with functional predictors and multiple scalar responses, with the help of regularization.

More recently, sparse regularization techniques have come to introduced to the functional regression models. Sparse regularization provides estimates some of which are exactly zeros and therefore is used for variable selection problems. Details of sparse regularization are described in Hastie et al. (2009) and Bühlmann and van de Geer (2011).

James et al. (2009) and Ferraty et al. (2010) applied the sparse regularization to the functional linear model and then selected time intervals of a functional predictor that truly affect the response. Matsui and Konishi (2011) applied the grouped sparse regularization (Yuan and Lin, 2006) to the functional linear model and selected variables in the framework of the functional linear models. The problem of functional regression modeling using ℓ_1-type regularization is considered in Aneiros et al. (2011), Zhao et al. (2012), Gertheiss et al. (2013) and Mingotti et al. (2013).

In this paper we consider the problem of variable selection for the multivariate linear model for functional data, a functional multivariate linear model. Advantages of our approach is that it captures the covariance structure between responses by treating them all together and that it can select functional predictors that affect the responses simultaneously. Matsui et al. (2008) estimated the model by the regularization method with an ℓ_2 type penalty. On the other hand, we apply an extension of the ℓ_1/ℓ_2 type penalty which is used for the multivariate linear models by Yuan et al. (2007) and Obozinski et al. (2011) in order to select variables given as functions appropriately in the multivariate linear model. We provide a coordinate descent algorithm (Friedman et al., 2007) for deriving estimators of the model by extending the result of Simon et al. (2013) which constructed the blockwise descent algorithm for estimating multivariate linear models. The estimated functional multivariate linear model is strongly affected by the value of a regularization parameter which control the degree of the penalty. In order to select its value appropriately we apply model selection criteria (Konishi and Kitagawa, 2008) for evaluating the estimated model. The effectiveness of the proposed estimation strategy is investigated through Monte Calro simulations. Furthermore, we apply it to the analysis of data on spectroscopy in order to select a set of variables that have a relationship to the contents of a meat sample.

The remainder of this paper is organized as follows. In Section 2 we briefly introduce the functional multivariate linear model and show that it is expressed as the classical multivariate linear model under certain assumptions. In section 3 we provide a method for estimating the functional multivariate linear model by the sparse regularization and model selection criteria for evaluating the estimated model. Monte Carlo simulations are conducted for verifying the effectiveness of the proposed method in Section 4, and then we apply the proposed method to the analysis of real data in Section 5. Finally we conclude the main points in Section 6.

2 Functional multivariate linear model

Suppose we have n observations with p predictors and K responses $\{(y_{ik}, x_{ij}(t));\ t \in \mathcal{T}_j,\ i = 1, \ldots, n,\ k = 1, \ldots, K, j = 1, \ldots, p\}$, where y_{ik} are scalar responses and $x_{ij}(t)$ are functional predictors. In addition, y_{ik} are supposed to be centered so that $\sum_{i=1}^{n} y_{ik} = 0$

for all k. Then we model the relationship between the responses and the predictors as

$$y_{ik} = \sum_{j=1}^{p} \int_{\mathcal{T}_j} x_{ij}(t)\beta_{jk}(t)dt + \varepsilon_{ik}, \tag{1}$$

where $\beta_{jk}(t)$ are coefficient functions and individual error vectors $\boldsymbol{\varepsilon}_i = (\varepsilon_{i1}, \ldots, \varepsilon_{iK})'$ are independent random vectors with mean vector $\mathbf{0}$ and unknown variance covariance matrix Σ.

We assume that the functional predictors $x_{ij}(t)$ are expressed as

$$x_{ij}(t) = \sum_{m=1}^{M_j} w_{ijm}\phi_{jm}(t) = \boldsymbol{w}_{ij}'\boldsymbol{\phi}_j(t), \tag{2}$$

where $\boldsymbol{w}_{ij} = (w_{ij1}, \ldots, w_{ijM_j})'$ are vectors of coefficients estimated by the penalized likelihood method. Details of this method are described in Araki et al. (2009). Several works such as Müller and Stadtmüller (2005) and Cai and Hall (2006) apply Karhunen-Loéve expansion that uses infinite dimensional orthonormal basis functions for functional data, while our method allows non-orthonormal basis such as B-splines or radial basis functions. In addition, derivatives of these data can be easily obtained by the expansion by calculating derivatives of basis functions. We also assume that $\beta_{jk}(t)$ are represented by linear combinations of M_j basis functions $\{\phi_{j1}(t), \ldots, \phi_{jM_j}(t)\}$, that is,

$$\beta_{jk}(t) = \sum_{m=1}^{M_j} b_{jkm}\phi_{jm}(t) = \boldsymbol{b}_{jk}'\boldsymbol{\phi}_j(t), \tag{3}$$

where $\boldsymbol{b}_{jk} = (b_{jk1}, \ldots, b_{jkM_j})'$ are vectors of coefficient parameters.

From assumptions (2) and (3), (1) can be rewritten by

$$y_{ik} = \sum_{j=1}^{p} \boldsymbol{w}_{ij}'\Phi_j\boldsymbol{b}_{jk} + \varepsilon_{ik}, \tag{4}$$

where $\Phi_j = \int_{\mathcal{T}_j} \boldsymbol{\phi}_j(t)\boldsymbol{\phi}_j(t)'dt$. Using the matrix representation, (4) can be expressed as

$$Y = \sum_{j=1}^{p} Z_{\cdot(j)}B_{(j)\cdot} + E, \tag{5}$$

where $Y = (y_{ik})_{ik}$ is an $n \times K$ matrix of responses, $Z_{\cdot(j)} = (\boldsymbol{z}_{1j}, \ldots, \boldsymbol{z}_{nj})'$ with $z_{ij} = \Phi_j\boldsymbol{w}_{ij}$, $B_{(j)\cdot} = (\boldsymbol{b}_{j1}, \ \ldots, \boldsymbol{b}_{jK})$, and $E = (\varepsilon_{ik})_{ik}$ is an $n \times K$ error matrix. Therefore, the problem of estimating $\beta_{jk}(t)$ in (1) can be regarded as that of estimating the parameter matrix $B = (B_{(1)\cdot}', \ldots, B_{(p)\cdot}')'$ in multivariate linear model (5).

3 Estimation via the sparse regularization

We estimate the parameter matrix B in (5) by the framework of the penalized least squared method. Consider the problem of minimizing the penalized squared error criterion

$$\frac{1}{2}\left\|Y - \sum_{j=1}^{p} Z_{\cdot(j)} B_{(j)\cdot}\right\|_F^2 + n\lambda \sum_{j=1}^{p} \hat{\rho}_j \left\|Z_{\cdot(j)} B_{(j)\cdot}\right\|_F \tag{6}$$

with respect to B, where $\|\cdot\|_F$ is a Frobenius norm, i.e., $\|A\|_F = \sqrt{\sum_i \sum_j a_{ij}^2}$ for $A = (a_{ij})_{ij}$ and $\hat{\rho}_j$ are products of weights $\sqrt{M_j}$ of the group lasso (Yuan and Lin, 2006) and adaptive weights $1/\|Z_{\cdot(j)}\hat{B}_{(j)\cdot}\|_F$ (Wang and Leng, 2008), here $\hat{B}_{(j)\cdot}$ are estimates obtained by minimizing (6) with $\hat{\rho}_j = \sqrt{M_j}$. Note that we applied the norm $\left\|Z_{\cdot(j)} B_{(j)\cdot}\right\|_F$ instead of $\left\|B_{(j)\cdot}\right\|_F$ as the penalty using the idea of the standardized group lasso (Simon and Tibshirani, 2012) in order to standardize the predictors. The criterion (6) corresponds to the penalized least squares criterion for the functional linear model (1) as follows:

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{k=1}^{K}\left(y_{ik} - \sum_{j=1}^{p} f_{jk}(x_{ij})\right)^2 + n\lambda \sum_{j=1}^{p} \hat{\rho}_j \left\{\sum_{i,k} f_{jk}(x_{ij})^2\right\}^{\frac{1}{2}},$$

where $f_{jk}(x_{ij}) = \int_{\mathcal{T}_j} x_{ij}(t)\beta_{jk}(t)dt$. Ravikumar et al. (2009) applied sparse regularization to the additive model with the idea of the standardized group lasso.

In order to obtain a minimizer of (6) we consider applying the coordinate descent algorithm. However, in general it is difficult to apply this algorithm directly unless $Z'_{\cdot(j)} Z_{\cdot(j)} = I$. In order to solve this problem, Simon et al. (2013) applied the QR decomposition to the design matrices in multivariate linear models. Suppose that the matrix for the j-th variable $Z_{\cdot(j)}$ is full rank. Then the QR decomposition gives $Z_{\cdot(j)} = Q_j R_j$, where Q_j is an $n \times M_j$ matrix each column of which are orthogonal, i.e. $Q_j' Q_j = I_{M_j}$, and R_j is an $M_j \times M_j$ upper triangular matrix. Using this decomposition and letting $\Theta_j = R_j B_{(j)\cdot}$, the penalized squared error (6) can be expressed as

$$\frac{1}{2}\left\|Y - \sum_{j=1}^{p} Q_j \Theta_j\right\|_F^2 + n\lambda \sum_{j=1}^{p} \hat{\rho}_j \left\|Q_j \Theta_j\right\|_F. \tag{7}$$

Since each column of Q_j are orthogonal, the norm $\|Q_j\Theta_j\|_F$ equals $\|\Theta_j\|_F$. Therefore it corresponds to the penalized squared error with design matrices Q_j that satisfy $Q_j'Q_j = I_j$.

The blockwise descent are performed in the following way. If the parameter matrices Θ_l for all $l \neq j$ were known, the problem of minimizing (7) would coincide with that of

$$\frac{1}{2}\left\|E_{-j} - Q_j\Theta_j\right\|_F^2 + n\lambda\hat{\rho}_j \left\|\Theta_j\right\|_F \tag{8}$$

with respect to Θ_j, where $E_{-j} = Y - \sum_{l \neq j} Q_l \Theta_l$ is a known matrix. The estimator $\hat{\Theta}_j$ of Θ_j satisfies the following equation by differentiating (8) with respect to Θ_j:

$$-Q_j' E_{-j} + \Theta_j + n\lambda\hat{\rho}_j D_j = O, \tag{9}$$

where D_j is given by

$$D_j = \begin{cases} \dfrac{\Theta_j}{\|\Theta_j\|_F} & (\Theta_j \neq O), \\ V_j \quad \text{s.t.} \quad \|V_j\|_F \leq 1 & (\Theta_j = O). \end{cases}$$

Equation (9) gives the estimator of Θ_j as

$$\hat{\Theta}_j = \left(1 - \frac{n\lambda\hat{\rho}_j}{\|Q_j' E_{-j}\|_F}\right)_+ Q_j' E_{-j},$$

where $(a)_+ = \max\{a, 0\}$ for $a \in \mathbb{R}$, and therefore the estimator of $B_{(j)\cdot}$ is given by $\hat{B}_{(j)\cdot} = R_j^{-1}\hat{\Theta}_j$. Putting it all together, the coordinate descent algorithm for the functional multivariate linear model is given as follows:

1. Apply the QR decomposition to $Z_{\cdot(j)}$ for all j: $Z_{\cdot(j)} = Q_j R_j$.
2. Assign initial values to $\Theta = (\Theta_1', \ldots, \Theta_p')'$ and let $E = Y - \sum_{j=1}^{p} Q_j \Theta_j$.
3. For $j = 1, \ldots, p$, calculate and update followings in order.
   (a) $E_{-j} = E + Q_j \Theta_j$.
   (b) $\hat{\Theta}_j = \left(1 - \dfrac{n\lambda\hat{\rho}_j}{\|Q_j' E_{-j}\|_F}\right)_+ Q_j' E_{-j}$.
   (c) $E = E_{-j} - Q_j \hat{\Theta}_j$.
4. Iterate Step 3 until convergence.
5. Calculate $\hat{B}_{(j)\cdot} = R_j^{-1}\hat{\Theta}_j$.

Then we have an estimated coefficient parameter $\hat{B} = (\hat{B}_{(1)\cdot}', \ldots, \hat{B}_{(p)\cdot}')'$, and an estimated variance covariance matrix $\hat{\Sigma} = (Y - Z\hat{B})(Y - Z\hat{B})'/n$.

Since the estimated model depends on the regularization parameter λ, we have to select these values appropriately. Typical criteria for selecting them include Akaike information criterion (AIC, Akaike, 1974) and Bayesian information criterion (BIC, Schwarz, 1978), which are respectively given by

$$\begin{aligned} \text{AIC} &= n \log |\hat{\Sigma}| + 2df(\lambda), \\ \text{BIC} &= n \log |\hat{\Sigma}| + df(\lambda) \log n, \end{aligned} \tag{10}$$

where $df(\lambda)$ is an effective degrees of freedom of the model and is given by

$$df(\lambda) = \sum_{j=1}^{p} \mathrm{tr}(S_j) I(\|\hat{\Theta}_j\|_F \neq 0), \quad S_j = Q_j \left(1 - \frac{n\lambda\hat{\rho}_j}{\|Q_j' E_{-j}\|_F}\right)_+ Q_j'.$$

This is due to the result of Ravikumar et al. (2009). Note that we abbreviate the terms that does not depend on λ in (10).

4 Simulation

We conducted Monte Carlo simulations in order to investigate the effectiveness of the proposed method. We simulated n sets of p predictors and K responses $\{(x_{ijs}, y_{ik}); i = 1, \ldots, n, \; j = 1, \ldots, p, \; s = 1, \ldots, n_{ij}, \; k = 1, \ldots, K\}$, where s denotes an index for the observed time point.

First, we constructed true coefficient functions as the following form:

$$\beta_{jk}(t) = \begin{cases} \sum_{m=1}^{6} \gamma_{jkm}\psi_{jm}(t) + \sum_{m=1}^{6} \delta_{jkm}\psi_{jm}(s) & j = 1, \ldots, p_0 \\ 0 & j = p_0 + 1, \ldots, p, \end{cases}$$

where $\gamma_{jkm} \sim^{iid} U(-3, 3)$, $\boldsymbol{\gamma}_{jk} = (\gamma_{jk1}, \ldots, \gamma_{jkM_j})'$, and $\boldsymbol{\delta}_{jk} = (\delta_{jk1}, \ldots, \delta_{jkM_j})'$ independently follows $N_{M_j}(\mathbf{0}, \Delta)$ with $\Delta_{xy} = 3\exp\{-0.5|x - y|\}$ and $\{\phi_{j1}(t), \ldots, \phi_{jM_j}(t)\}$ are Gaussian radial basis functions given by Kawano and Konishi (2007). This indicates that only the first p_0 variables are relevant to the response. Then we simulated predictors and responses for 100 times in following ways. The longitudinal predictors x_{ijs} are obtained from discretized time points t_s as follows:

$$\begin{aligned} x_{ijs} &= u_{ij}(t_s) + \varepsilon_{ijs}^{(x)}, \\ u_{ij}(t) &= \sum_{m=1}^{6} \alpha_{jm}\psi_{jm}(t) + \sum_{m=1}^{6} \beta_{ijm}\psi_{jm}(t) = (\boldsymbol{\alpha}_j + \boldsymbol{\beta}_{ij})'\boldsymbol{\psi}_j(t), \end{aligned}$$

where $\varepsilon_{ijs}^{(x)}$ independently follow $N(0, 0.3R_{ij}^{(x)})$ with $R_{ij}^{(x)} = \max_s\{u_{ij}(t_s)\} - \min_s\{u_{ij}(t_s)\}$, $\alpha_{jm} \sim^{iid} U(-10, 10)$, $\boldsymbol{\alpha}_j = (\alpha_{j1}, \ldots, \alpha_{jM_j})'$, $\boldsymbol{\beta}_{ij} = (\beta_{ij1}, \ldots, \beta_{ijM_j})'$ independently follow $N_{M_j}(\mathbf{0}, \Omega)$ with $\Omega_{xy} = 2\exp\{-0.5|x - y|\}$ and $\boldsymbol{\psi}_j(t) = (\phi_{j1}(t), \ldots, \phi_{jM_j}(t))'$. Then we have responses y_{ik} by

$$\begin{aligned} y_{ik} &= f_{ik} + \varepsilon_{ik}, \\ f_{ik} &= \sum_{j=1}^{p} \int u_{ij}(t)\beta_{jk}(t)dt = \sum_{j=1}^{p} (\boldsymbol{\alpha}_j + \boldsymbol{\beta}_{ij})'\Psi_j(\boldsymbol{\gamma}_{jk} + \boldsymbol{\delta}_{jk}), \end{aligned}$$

where $\boldsymbol{\varepsilon}_i = (\varepsilon_{i1}, \ldots, \varepsilon_{iK})' \sim^{iid} N_K(\mathbf{0}, \Sigma)$ with $\Sigma_{kl} = 0.3R_kR_l\exp\{-0.5|k - l|\}$ with $R_k = \max_i\{f_{ik}\} - \min_i\{f_{ik}\}$ and $\Psi_j = \int \boldsymbol{\psi}_j(t)\boldsymbol{\psi}_j(t)'dt$.

We assumed the number of time points $s_{ij} = 30$ for all i, j, the number of responses $K = 2$ and the number of relevant predictors to the responses $p_0 = p/2$, and then examined for several values for the sample size $n = 100, 200$, the number of variables $p = 10, 20$. We analyzed this data set for cases using AIC and BIC given in (10), and with adaptive weights $1/\|Z_{\cdot(j)} B_{(j)\cdot}\|_F$ in (6) and without ones. We also compared the method for multivariate linear models with that for univariate ones. We then evaluated following averaged values for 100 repetitions to evaluate the effectiveness of the proposed method in several viewpoints. In order to evaluate the prediction accuracy of the estimated model, we calculated averages of mean squared errors and the Kullback-Leibler (KL) information between the true and estimated model, respectively given by

$$\mathrm{MSE}_k = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_{ik} - f_{ik})^2,$$
$$\mathrm{KL} = \frac{n}{2}\log\frac{\hat{\Sigma}}{\Sigma} + \frac{1}{2}\mathrm{tr}\left\{(F-\hat{Y})\hat{\Sigma}^{-1}(F-\hat{Y})\right\} - \frac{nK}{2} + \frac{n}{2}\mathrm{tr}\left\{\Sigma\hat{\Sigma}^{-1}\right\},$$

where $F = (f_{ik})_{ik}$ and $\hat{Y} = (\hat{y}_{ik})_{ik}$ is the predicted values of Y. In order to investigate the accuracy of model selection we investigated 100 averages of true and false positive rates respectively defined by

$$\mathrm{TPR}_k = \frac{1}{p_0}\sum_{j=1}^{p_0} I(\hat{\beta}_{jk}(t) \neq 0),$$
$$\mathrm{FPR}_k = \frac{1}{p-p_0}\sum_{j=p_0+1}^{p} I(\hat{\beta}_{jk}(t) \neq 0).$$

where $I(\cdot)$ is an indicator function and $\hat{\beta}_{jk}(t)$ are estimated coefficient functions.

The results are shown in Tables 1 and 2. I may be seen from these results that the proposed method minimize MSEs and KLs the most. In particular, the models evaluated by AIC are superior to those based on BIC. The proposed method for the multivariate linear model tends to select more variables than that for the univariate model. Furthermore, the models with BIC and adaptive weights tends to select fewer variables than those with other settings, and therefore they give lower TPRs and FPRs. The proposed method with AIC and adaptive weights give relatively higher TPRs and lower FPRs.

5 Real data analysis

We applied the proposed method to the analysis of spectrometric data, available from StatLib Data Archive (http://lib.stat.cmu.edu/datasets/tecator). The absorbance of near-infrared spectra of a meat sample are observed at equal intervals with 100 channels from the wavelength range of from 850 nm to 1,050 nm. The spectra are considered to be associated with contents of the meat sample such as water, fat, and protein, and therefore an objective of our analysis is to model the relationship between them.

The analysis of spectrometric data have been widely studied. For example, Rossi et al. (2005) approached this problem using a B-spline approximation and modeling based on neural networks to predict the fat content, and then Matsui et al. (2008) applied the functional multivariate linear model to the analysis of it in order to incorporate information of all three contents of the meat sample. On the other hand, Goutis (1998) suggested that the second derivative of the spectra is important since it annihilates the linear shift induced in the observation, and then constructed a functional linear model where the predictor is a second derivative of a function of the spectra. Here we treated several orders of derivatives of functions of spectra all together, and then investigated which combinations of them contribute to the contents of meat sample. Furthermore, we treated all three contents simultaneously and then applied the functional multivariate linear model.

The flow of the analysis is as follows. First, we obtained standardized data set by subtracting a sample mean and dividing a sample standard deviations for each time points. Then we converted observed longitudinal data into functional data by the basis function expansion approach. We also constructed several orders of derivatives of functional data by obtaining derivatives of basis functions. Details of obtaining derivatives of functional data are given in Appendix. Note that Ramsay and Silverman (2005), chapter 3 notes that when we require the n-th derivatives of functional data, we should penalize the derivatives of order $n + 2$ rather than the second order ones in the process of converting longitudinal data into functions. In this case we have to apply the smoothing techniques for all derivatives, while our method reduces computational burden by smoothing the original data. Examples of functional data and their derivatives are given in Figure 1. Next we constructed the functional multivariate linear model and then estimated by the proposed method, here we used the model selection criterion AIC. We repeated this analysis for 200 bootstrap samples, and then investigated the number of selected functional variables.

The result on variable selection is given in Table 3. The proposed method selected functional predictors appropriately, and this table suggested that the original, first and second derivatives of the spectra affect the contents of the meat sample. Table 4 shows training and test errors for the proposed method and the functional univariate linear model. The test errors of our method are competitive to the existing method.

6 Concluding Remarks

We have considered an estimation procedure for the functional linear model with multiple functional predictors and scalar responses. Since there are multiple parameters for one predictor, we applied the ℓ_1/ℓ_2 type regularization to the model that appropriately select these predictors. The estimators of the model are obtained through coordinate descent algorithm by extending existing ones, and then tuning parameters included in the model were selected by information criteria. In order to confirm the effectiveness of the proposed method we applied it to the analysis of spectrometric data, and then modeled the relationship between the functions of the absorbance of spectra and contents of meat sample. Results showed that the proposed method gave adequate results in viewpoints of prediction and model selection accuracy.

In this work we do not consider any interactions between predictors. On the other hand, Fuchs et al. (2015) considered functional regression models with interactions. The extension of our method to the case with interactions can be considered, but is a topic for future works.

Appendix

Basis functions

In this paper we consider using Gaussian radial basis functions (RBF) for basis functions $\boldsymbol{\phi}_j(t) = (\phi_{j1}(t), \ldots, \phi_{jM_j}(t))'$ in (2) and (3). It is given by

$$\phi_{jm}(t) = \exp\left\{-\frac{(t-\mu_{jm})^2}{\sigma_{jm}^2}\right\},$$

where μ_{jm} and σ_{jm}^2 respectively represent center and dispersion parameters. Kawano and Konishi (2007) decided these parameters using the idea of B-splines.

The 1st derivative of the RBF $\phi_{jm}(t)$ is given by

$$\phi_{jm}^{(1)}(t) = -\frac{t-\mu_{jm}}{\sigma_m^2}\phi_m(t).$$

Then the $(n+2)$-th derivative of RBF is recursively obtained by

$$\phi_{jm}^{(n+2)}(t) = -\frac{n+1}{\sigma^2}\phi_{jm}^{(n)}(t) - \frac{x-\mu}{\sigma^2}\phi_{jm}^{(n+1)}(t).$$

The n-th derivative of a functional data $x(t)$ can be expressed by $x^{(n)}(t) = \hat{\boldsymbol{w}}'\boldsymbol{\phi}^{(n)}(t)$ where $\boldsymbol{\phi}^{(n)}(t) = (\phi_1^{(n)}(t), \ldots, \phi_M^{(n)}(t))'$. Therefore, if we use the $(j-1)$-th derivative of the functional data $x^{(j-1)}(t)$ as the j-th predictor, the functional linear model (1) is given by

$$\begin{aligned} y_{ik} &= \sum_{j=1}^{p}\int_{\mathcal{T}} x_i^{(j-1)}(t)\beta_{jk}(t)dt + \varepsilon_{ik} \\ &= \sum_{j=1}^{p}\boldsymbol{w}_i'\int_{\mathcal{T}}\boldsymbol{\phi}^{(j-1)}(t)\boldsymbol{\phi}_j(t)'dt\boldsymbol{b}_{jk} + \varepsilon_{ik} \\ &= \sum_{j=1}^{p}\boldsymbol{w}_i'\Phi^{(j)}\boldsymbol{b}_{jk}, \end{aligned}$$

where $\Phi^{(j)} = \int_{\mathcal{T}}\boldsymbol{\phi}^{(j)}(t)\boldsymbol{\phi}_j(t)'dt$.

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Table 1: Results on simulation studies for $n = 100$. Values are averages of 100 repetitions and standard deviations (in brackets), the notation "adapt." indicates the results with the adaptive weights and $\#_k$ are numbers of selected variables for the k-th response.

	Multivariate (proposed)				Univariate			
	AIC	BIC	AIC (adapt.)	BIC (adapt.)	AIC	BIC	AIC (adapt.)	BIC (adapt.)
$p = 10$, $p_0 = 5$								
MSE_1	194.48 (45.58)	208.17 (65.19)	83.76 (30.07)	120.28 (77.99)	256.15 (54.28)	259.09 (57.04)	142.19 (55.70)	164.39 (68.84)
MSE_2	182.57 (48.13)	195.33 (67.42)	76.19 (21.65)	103.73 (63.48)	216.77 (59.09)	218.67 (63.74)	104.57 (41.13)	112.02 (53.77)
KL	207.31 (16.54)	211.79 (22.41)	141.99 (16.71)	159.01 (32.67)	234.61 (18.29)	234.99 (18.49)	208.50 (66.29)	206.17 (52.21)
$\#_1$	5.74 (1.36)	5.40 (1.39)	5.48 (1.40)	4.35 (1.42)	3.22 (1.36)	3.10 (1.33)	3.06 (1.35)	2.41 (1.13)
$\#_2$	5.74 (1.36)	5.40 (1.39)	5.48 (1.40)	4.35 (1.42)	3.17 (1.16)	3.13 (1.17)	3.05 (1.18)	2.67 (1.08)
TPR_1	89.80 (11.55)	85.80 (15.90)	89.20 (11.86)	75.20 (19.92)	52.40 (17.93)	51.60 (18.02)	52.20 (18.62)	44.60 (19.66)
TPR_2	89.80 (11.55)	85.80 (15.90)	89.20 (11.86)	75.20 (19.92)	49.80 (14.91)	49.60 (14.63)	50.40 (14.90)	46.60 (14.79)
FPR_1	25.00 (23.51)	22.20 (22.54)	20.40 (23.26)	11.80 (16.84)	12.00 (17.06)	10.40 (15.43)	9.00 (15.67)	3.60 (9.16)
FPR_2	25.00 (23.51)	22.20 (22.54)	20.40 (23.26)	11.80 (16.84)	13.60 (18.18)	13.00 (17.84)	10.60 (16.93)	6.80 (13.09)
$p = 20$, $p_0 = 10$								
MSE_1	286.78 (58.33)	480.78 (134.27)	95.36 (26.15)	413.55 (178.02)	366.32 (86.99)	402.72 (99.51)	187.02 (79.15)	355.44 (168.14)
MSE_2	250.42 (60.45)	406.34 (114.94)	87.62 (33.23)	361.31 (154.08)	332.21 (78.15)	350.31 (95.79)	177.33 (73.55)	328.41 (149.87)
KL	224.51 (17.11)	267.62 (20.47)	163.80 (24.01)	249.36 (41.10)	258.67 (18.67)	260.71 (17.42)	325.39 (107.69)	257.21 (30.63)
$\#_1$	11.39 (2.26)	7.31 (2.06)	11.33 (2.34)	3.92 (2.26)	7.19 (3.12)	6.35 (2.45)	6.87 (3.08)	3.44 (2.11)
$\#_2$	11.39 (2.26)	7.31 (2.06)	11.33 (2.34)	3.92 (2.26)	6.25 (2.48)	5.78 (2.25)	5.90 (2.43)	2.89 (2.13)
TPR_1	81.90 (10.80)	55.40 (15.14)	81.60 (10.80)	29.00 (21.44)	52.90 (18.11)	48.50 (16.35)	52.00 (17.87)	29.50 (16.72)
TPR_2	81.90 (10.80)	55.40 (15.14)	81.60 (10.80)	29.00 (21.44)	49.50 (16.54)	47.10 (16.65)	48.00 (16.70)	25.60 (18.11)
FPR_1	32.00 (20.55)	17.70 (16.01)	31.70 (21.23)	10.20 (11.55)	19.00 (17.95)	15.00 (14.18)	16.70 (17.29)	4.90 (9.04)
FPR_2	32.00 (20.55)	17.70 (16.01)	31.70 (21.23)	10.20 (11.55)	13.00 (14.18)	10.70 (12.08)	11.00 (12.59)	3.30 (6.04)

Table 2: Results on simulation studies for $n = 200$. Values are averages of 100 repetitions and standard deviations (in brackets), the notation "adapt." indicates the results with the adaptive weights and $\#_k$ are numbers of selected variables for the k-th response.

	Multivariate (proposed)				Univariate			
	AIC	BIC	AIC (adapt.)	BIC (adapt.)	AIC	BIC	AIC (adapt.)	BIC (adapt.)
	$p = 10$, $p_0 = 5$							
MSE_1	139.32 (35.38)	154.14 (50.23)	83.37 (25.58)	98.98 (43.17)	155.47 (42.06)	159.21 (46.12)	92.67 (27.72)	108.10 (38.93)
MSE_2	133.06 (33.38)	145.39 (41.57)	81.19 (21.77)	93.66 (33.98)	144.70 (40.75)	146.82 (41.77)	93.30 (26.15)	101.65 (30.92)
KL	345.69 (28.34)	359.01 (37.37)	268.25 (32.63)	284.78 (46.28)	369.84 (29.78)	371.93 (31.08)	301.94 (30.43)	316.98 (37.10)
$\#_1$	7.29 (1.51)	6.38 (1.33)	6.12 (1.21)	5.05 (1.10)	5.38 (1.50)	5.07 (1.38)	5.13 (1.28)	4.04 (1.09)
$\#_2$	7.29 (1.51)	6.38 (1.33)	6.12 (1.21)	5.05 (1.10)	4.08 (1.42)	3.87 (1.26)	3.85 (1.34)	3.06 (0.99)
TPR_1	100.00 (0.00)	98.40 (5.45)	99.80 (2.00)	89.80 (12.23)	89.80 (12.55)	87.20 (14.36)	89.40 (12.21)	75.40 (16.29)
TPR_2	100.00 (0.00)	98.40 (5.45)	99.80 (2.00)	89.80 (12.23)	69.20 (16.68)	67.20 (15.96)	68.00 (16.08)	57.00 (14.60)
FPR_1	45.80 (30.26)	29.20 (25.01)	22.60 (23.89)	11.20 (17.37)	17.80 (22.54)	14.20 (20.16)	13.20 (18.47)	5.40 (11.32)
FPR_2	45.80 (30.26)	29.20 (25.01)	22.60 (23.89)	11.20 (17.37)	12.40 (19.02)	10.20 (16.94)	9.00 (17.61)	4.20 (11.12)
	$p = 20$, $p_0 = 10$							
MSE_1	212.08 (37.85)	364.73 (99.05)	109.42 (26.03)	240.90 (126.86)	250.06 (57.71)	330.53 (103.01)	135.53 (30.13)	240.87 (98.45)
MSE_2	177.53 (29.73)	306.47 (78.41)	93.14 (17.33)	215.34 (125.31)	216.65 (39.58)	259.14 (63.01)	125.39 (25.26)	196.11 (72.68)
KL	376.25 (25.00)	467.74 (45.49)	279.41 (21.94)	382.73 (86.10)	424.97 (29.16)	457.66 (39.52)	371.30 (48.20)	426.92 (49.33)
$\#_1$	15.27 (2.12)	9.04 (1.83)	13.68 (3.10)	7.28 (2.46)	10.21 (2.03)	7.14 (1.83)	9.92 (2.12)	5.39 (1.90)
$\#_2$	15.27 (2.12)	9.04 (1.83)	13.68 (3.10)	7.28 (2.46)	9.09 (1.97)	6.73 (1.60)	8.70 (2.12)	5.19 (1.81)
TPR_1	97.30 (4.68)	78.50 (13.13)	96.40 (5.03)	66.60 (22.48)	81.50 (11.14)	63.90 (14.21)	80.90 (11.11)	50.30 (17.08)
TPR_2	97.30 (4.68)	78.50 (13.13)	96.40 (5.03)	66.60 (22.48)	73.80 (11.17)	60.50 (12.98)	72.20 (11.68)	48.30 (15.70)
FPR_1	55.40 (20.02)	11.90 (14.05)	40.40 (27.96)	6.20 (11.44)	20.60 (15.82)	7.50 (10.48)	18.30 (15.83)	3.60 (6.74)
FPR_2	55.40 (20.02)	11.90 (14.05)	40.40 (27.96)	6.20 (11.44)	17.10 (14.93)	6.80 (7.90)	14.80 (13.96)	3.60 (6.44)

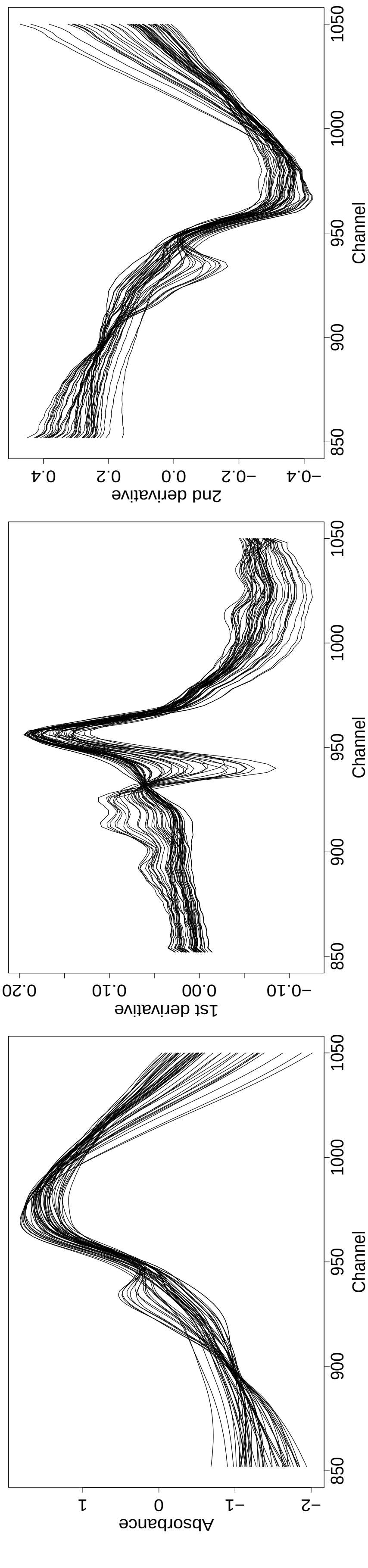

Figure 1: 100 examples of functions of absorbance spectra (left), their 1st derivatives (center) and 2nd derivatives (right).

Table 3: Results on variable selection for the analysis of spectrometric data. Numbers 0th to 9th indicate orders of derivatives of predictors.

Predictor		0th	1st	2nd	3rd	4th	5th	6th	7th	8th	9th
Multivariate		200	200	175	2	0	0	0	0	0	0
Univariate	Water	199	195	94	1	0	0	0	0	1	0
	Fat	200	124	122	118	0	0	0	0	0	0
	Protein	198	199	196	123	25	16	7	2	1	1

Table 4: Result on training and test errors for the analysis of spectrometric data.

	Multivariate		Univariate	
	Train	Test	Train	Test
Water	1.265 (0.200)	6.337 (2.248)	1.507 (0.206)	6.284 (2.227)
Fat	1.647 (0.267)	8.269 (3.182)	2.095 (0.803)	8.359 (3.126)
Protein	0.172 (0.025)	0.576 (0.270)	0.381 (0.063)	0.654 (0.236)

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