

A Simulation Study of Functional Density-Based Inverse Regression

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Abstract

In this paper a new nonparametric functional method is introduced for predicting a scalar random variable Y on the basis of a functional random variable X . The prediction has the form of a weighted average of the training data y_i , where the weights are determined by the conditional probability density of X given $Y = y_i$, which is assumed to be Gaussian. In this way such a conditional probability density is incorporated as a key information into the estimator. Contrary to some previous approaches, no assumption about the dimensionality of $E(X|Y = y)$ or about the distribution of X is required. The new proposal is computationally simple and easy to implement. Its performance is assessed through a simulation study.

1 Introduction

The fast development of instrumental analysis equipment and modern measurement devices provides huge amounts of data as high-resolution digitized functions. As a consequence, Functional Data Analysis (FDA) has become a growing research field [1, 2]. In the FDA setting, each individual is treated as a single entity described by a continuous real-valued function rather than by a finite-dimensional vector: functional data (FD) are then supposed to have values in an infinite dimensional space, typically a Hilbert space \mathcal{X} with scalar product $\langle \cdot, \cdot \rangle$.

Specifically, in functional regression analysis one intends to predict a random scalar variable (response variable) Y from a functional random variable (predictor) X (e.g., with values in $\mathcal{X} = L_2([a, b])$). That is, the goal is to estimate the regression function $\gamma(x) = \mathbb{E}(Y|X = x)$, where $\mathbb{E}(Y|X)$ denotes the conditional expectation, on the basis of a sample $(x_i, y_i)_{i=1, \dots, n}$ of independent realizations

of (X, Y) . Equivalently, the aim is to fit the functional regression model

$$Y = \gamma(X) + \epsilon,$$

where ϵ is a real random variable independent of X . Several approaches have been proposed for this problem, which can be classified into three main families:

- a) *Linear regression methods.* Earlier work were focused on linear regression models where the regression function γ takes the linear form

$$\gamma(x) = c + \langle \beta, x \rangle,$$

where $c \in \mathbb{R}$ and $\beta \in \mathcal{X}$ are unknown parameters. A review of approaches for estimating this model can be found in [1]; see also, [3, 4, 5, 6, 7, 8, 9].

- b) *Nonparametric regression methods.* A drawback of linear regression methods is that they can not deal with nonlinear dependencies between the predictor and the response variables. To overcome this, a number of nonparametric approaches has been proposed. We review the most important approaches developed in the past few years in that area.

The first approach, introduced in [2], is the use of functional kernel regression estimators:

$$\hat{\gamma}(x) = \frac{\sum_{i=1}^n K(d(x_i, x)/h)y_i}{\sum_{i=1}^n K(d(x_i, x)/h)},$$

where $h > 0$ is the kernel bandwidth, d is a semi-metric on \mathcal{X} and $K : R_+ \rightarrow R$ is a suitable kernel function. This kind of estimators allows for great flexibility in fitting nonlinear models. However, their consistency properties have been demonstrated only for restricted classes of kernel functions such as those of types I and II in [2]; furthermore, the data-driven selection of the kernel bandwidth h is a difficult problem, especially for this high dimensional setting.

Another class of nonparametric regression estimators are the Functional Neural Networks proposed by Rossi et. al. [10]. In particular, the single hidden layer perceptron is defined by

$$\hat{\gamma}(x) = \sum_{j=1}^q \hat{a}_j T(\hat{u}_j + \hat{l}_j(x)),$$

where $T : R \rightarrow R$ is a given activation function, $(l_j)_j$ are unknown linear functionals to be estimated (e.g., $l_j(x) = \langle w_j, x \rangle$ with $w_j \in \mathcal{X}$) and $(a_j)_j$, $(u_j)_j \subset \mathbb{R}$ are unknown parameters that also have to be estimated. Functional perceptrons have the universal approximation property that makes it possible to represent a wide variety of nonlinear functionals. But notice that they depend on a quite large number of parameters $(w_j)_j$, $(a_j)_j$, $(u_j)_j$, which greatly increases with the number of neurons, q , and that their estimation by the optimization of the least square error leads to local minima issues. Also,

the number of neurons has to be tuned which is a computationally difficult task. In the same spirit, functional versions of the radial basis functions neural networks have been introduced in [11].

Also, the general framework of function approximation in Reproducing Kernel Hilbert Spaces (RKHS) has been used [12, 13] to introduce functional regression estimators, which have the general form:

$$\hat{\gamma}(x) = \sum_{i=1}^n \hat{a}_i K(x_i, x),$$

where K is a reproducing kernel on \mathcal{X} , and $(a_i)_i \in \mathbb{R}$. In this framework can be included functional versions of support vector regression [13] and radial basis functions [12]. The latter has the specific form:

$$\hat{\gamma}(x) = \sum_{i=1}^m \hat{a}_i \phi(d(x, c_i)),$$

where ϕ is the adopted radial basis function, $c_1, \dots, c_m \in \mathcal{X}$ are given centers, d is a distance defined on \mathcal{X} , and $(a_i)_i$ are unknown parameters.

An important advantage of the RKHS approach is that the resulting estimator is linear with respect to the unknown parameters $(a_i)_i$: their estimation by least squares optimization thus reduces to solve an algebraic linear problem. However, contrary to standard RKHS methods for approximating multivariate functions (e.g., standard multivariate splines and radial basis functions such as thin-plate splines), in the FDA setting the smoothness properties of $\hat{\gamma}$ as a functional on \mathcal{X} have not been yet defined. Hence, the selection of suitable reproducing kernels and radial basis functions is still an open issue.

Finally, more recently, k -nearest neighbors regression has been generalized to functional data [14, 15]. This approach leads to the following regression function:

$$\hat{\gamma}(x) = \frac{1}{k} \sum_{i=1}^k y_{(i,x)}$$

where $y_{(i,x)}$ is the value of Y for the i -th nearest neighbors of x among $(x_i)_{i=1, \dots, n}$. The consistency, as well as a rate of convergence, is given for this approach, depending on regularity conditions on γ .

- c) *Functional Inverse Regression (FIR) methods.* More recently, an alternative methodology has been introduced that can be regarded as a compromise between too restrictive parametric methods (such as linear regression) and nonparametric ones (such as kernel methods). This is called Functional Inverse Regression (FIR or FSIR) [16, 17, 18], and constitutes a functional version of the Sliced Inverse Regression (SIR) previously proposed for multivariate regression models [19]. The FIR approach assumes that the following model holds:

$$Y = g(\langle \beta_1, X \rangle, \dots, \langle \beta_d, X \rangle) + \epsilon,$$

where d is the so-called effective dimension and $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is an unknown function. Under some additional assumptions (which are guaranteed if X has an elliptic distribution, e.g., a Gaussian distribution in the Hilbert space \mathcal{X}) the directions $(\beta_j)_j$ can be estimated from the spectral decomposition of the covariance operators $\mathbb{V}(X)$ and $\mathbb{V}(\mathbb{E}(X|Y))$. The latter involves to fit the mean function of the “inverse” model

$$X = \mu(Y) + e, \quad (1)$$

where e is a random element in \mathcal{X} with zero mean, not correlated with Y . More specifically, to estimate $(\beta_j)_j$ and g , the following steps are carried out:

1. Obtain an estimate of $\mu(Y) = \mathbb{E}(X|Y)$ by regressing each component of X versus Y through any univariate nonparametric regression method.
2. Obtain estimates of the covariance operators $\Gamma = \mathbb{V}(X)$ and $\Gamma_e = \mathbb{V}(\mathbb{E}(X|Y))$ on the basis of the results of step (1), and carry out the spectral decomposition of the operator $\Gamma^{-1/2}\Gamma_e\Gamma^{-1/2}$. $(\beta_j)_j$ are estimated as the eigenfunctions corresponding to the d first greatest eigenvalues.
3. Finally, estimate g through a d -variate nonparametric regression method.

In this semi-parametric approach, the dimension, d , is an hyper-parameter of the model. Several methods have been proposed to find a good d , such as the one proposed in [20].

In this paper, a new functional regression method to estimate $\gamma(X)$ is introduced that also relies on regarding the inverse regression model (1). Its main practical motivation arises from calibration problems in Chemometrics, specifically in spectroscopy, where some chemical variable Y (e.g., concentration) needs to be predicted from a digitized function X (e.g., an spectrum). In this setting, said “inverse” model represents the physical data generation process in which the output spectrum X is determined by the input chemical concentration Y , and e is a functional random perturbation mainly due to the measurement procedure. Though Y and X could have unknown complex probability distributions, it is a common assumption that the perturbation e follows a Gaussian distribution P_0 , and so that the conditional distribution $P(\cdot/y)$ of X given $Y = y$ is a Gaussian distribution on \mathcal{X} with mean $\mu(y)$. This suggests the following estimate of $\gamma(x)$:

$$\hat{\gamma}(x) = \frac{\sum_{i=1}^n \hat{f}(x/y_i) y_i}{\hat{f}_X(x)},$$

where $\hat{f}(x/y)$ is an estimate of the density $f(x/y)$ of $P(\cdot/y)$ with respect to the measure P_0 . This regression estimate will be referred to as functional Density-Based Inverse Regression (DBIR). If X was a scalar variable, this would reduce to the approach for univariate calibration proposed in [21]. It requires more specific assumptions about the distribution of the perturbation e in the inverse model (1) (e.g., Gaussian distribution) but it has a number of appealing features in comparison with other approaches:

- Likewise other nonparametric approaches, it allows one to capture *non-linear regression functions*.
- Likewise the FIR approach it requires to estimate the mean function μ of the inverse model and some covariance operator (specifically, $\mathbb{V}(e)$). μ should be estimated through a nonparametric regression method but, contrary to the classical nonparametric functional regression, this function is defined on \mathbb{R} (and not in an infinite dimensional Hilbert space) and the estimation task is thus much easier, as well as the issue of tuning the hyperparameters (if so) in the chosen nonparametric regression method. Moreover, no other parameter has to be estimated. In particular, unlike functional kernel regression, this approach does not require the selection of the bandwidth for a kernel on an infinite dimensional space. Also, it does not involve a large number of parameters related in a non quadratic way to the functional to optimize, contrary to, e.g., the case of functional perceptrons. DBIR is thus *computationally very easy to use*.
- Finally, unlike the FIR approach, *few assumptions are required*: in particular, γ does not need to be a function of a finite number d of projections nor X has to follow an elliptical distribution (or any other given distribution). Also notice that DBIR does not require the additional multivariate nonparametric fitting step (c) aforementioned.

This paper is organized as follows. Section 2 defines the functional Density-Based Inverse Regression (DBIR) estimator. Section 3 carries out a simulation study in order to assess the feasibility and performance of the DBIR method. Finally, some conclusions are given in Section 4.

2 Functional Density-Based Inverse Regression (DBIR)

2.1 Definition of DBIR in an abstract setting

Let (X, Y) be a pair of random variables taking values in $\mathcal{X} \times \mathbb{R}$ where $(\mathcal{X}, \langle \cdot, \cdot \rangle)$ is the space of square integrable functions from \mathbb{R} to \mathbb{R} ($\mathcal{X} = L^2([a, b])$). Suppose also that n i.i.d. realizations of (X, Y) are given, denoted by $(x_i, y_i)_{i=1, \dots, n}$. The goal is to build, from $(x_i, y_i)_i$, a predictor of the value of Y corresponding to a future observed value of X . This problem is usually addressed through the estimation of the regression function $\gamma(x) = \mathbb{E}(Y|X = x)$.

For this, the functional Density-Based Inverse Regression (DBIR) approach fits the inverse regression model:

$$X = F(Y) + \epsilon, \tag{2}$$

where ϵ is a random process (perturbation or noise) with zero mean, independent of Y , and $y \rightarrow F(y)$ is a function from \mathbb{R} into \mathcal{X} . As was stated in Section 1,

this is the commonly assumed data generating model in calibration problems [22].

Additionally, the following assumptions are made:

1. it exists a probability measure P_0 on \mathcal{X} (not depending on y) such that the conditional probability measure of X given $Y = y$, say $P(\cdot/y)$, has a density $f(\cdot/y)$ with respect to P_0 ; i.e.,

$$P(A/y) = \int_A f(x/y) P_0(dx)$$

for any measurable set A in \mathcal{X} ;

2. it is assumed that Y is a continuous random variable, i.e., its distribution has a density $f_Y(y)$ (with respect to the Lebesgue measure on \mathbb{R}).

Under these assumptions, the regression function can be written

$$\gamma(x) = \frac{\int_{\mathbb{R}} f(x/y) f_Y(y) y dy}{f_X(x)},$$

where

$$f_X(x) = \int_{\mathbb{R}} f(x/y) f_Y(y) dy.$$

Hence, given an estimate $\hat{f}(x/y)$ of $f(x/y)$, the following (plug-in) estimate of $\gamma(x)$ can be constructed from the previous equation:

$$\hat{\gamma}(x) = \frac{\sum_{i=1}^n \hat{f}(x/y_i) y_i}{\hat{f}_X(x)}, \quad (3)$$

where

$$\hat{f}_X(x) = \sum_{i=1}^n \hat{f}(x/y_i).$$

2.2 Specification in the Gaussian case

The general estimator given in Equation (3) will be here specified for the case where, for each $y \in \mathbb{R}$, $P(\cdot/y)$ is a Gaussian measure on $\mathcal{X} = \mathcal{L}_2[0, 1]$. $P(\cdot/y)$ is then determined by its corresponding mean function $\mu(y) \in \mathcal{X}$ (which is then equal to $F(y)$ according to Equation (2)) and a covariance operator r (not depending on y), which is a symmetric and positive Hilbert-Schmidt operator on the space \mathcal{X} . Thus, there exists an eigenvalue decomposition of r , $(\varphi_j, \lambda_j)_{j \geq 1}$ such that $(\lambda_j)_j$ is a decreasing sequence of positive real numbers, $(\varphi_j)_j$ take values in \mathcal{X} and $r = \sum_j \lambda_j \varphi_j \otimes \varphi_j$ where $\varphi_j \otimes \varphi_j(h) = \langle \varphi_j, h \rangle \varphi_j$ for any $h \in \mathcal{X}$.

Denote by P_0 the Gaussian measure on \mathcal{X} with zero mean and covariance operator r . Assume that the following usual regularity condition holds: for each $y \in \mathbb{R}$,

$$\sum_{j=1}^{\infty} \frac{\mu_j^2(y)}{\lambda_j} < \infty,$$

where

$$\mu_j(y) = \langle \mu(y), \varphi_j \rangle.$$

Then, $P(\cdot/y)$ and P_0 are equivalent Gaussian measures, and the density $f(\cdot/y)$ has the explicit form:

$$f(x/y) = \exp \left\{ \sum_{j=1}^{\infty} \frac{\mu_j(y)}{\lambda_j} \left(x_j - \frac{\mu_j(y)}{2} \right) \right\},$$

where $x_j = \langle x, \varphi_j \rangle$ for all $j \geq 1$. This leads to the following algorithm to estimate $f(x/y)$:

1. Obtain an estimate $\hat{\mu}(\cdot)(t)$ of the function $y \rightarrow \mu(y)(t)$ for each $t \in \mathbb{R}$. This may be carried out through any standard nonparametric method for univariate regression based on the data set $(y_i, x_i(t))_{i=1, \dots, n}$, e.g., a smoothing kernel method:

$$\hat{\mu}(y) = \frac{\sum_{i=1}^n K\left(\frac{y_i - y}{h}\right) x_i}{\sum_{i=1}^n K\left(\frac{y_i - y}{h}\right)} \quad (4)$$

as proposed in [23] (note that, in this case, the bandwidth h has a common value for all t).

2. Obtain estimates $(\hat{\varphi}_j, \hat{\lambda}_j)_j$ of the eigenfunctions and eigenvalues $(\varphi_j, \lambda_j)_j$ of the covariance r on the basis of the empirical covariance of the residuals $\hat{e}_i = x_i - \hat{\mu}(y_i)$, $i = 1, \dots, n$

$$\hat{r} = \frac{1}{n} \sum_{i=1}^n (\hat{e}_i - \bar{e}) \otimes (\hat{e}_i - \bar{e})$$

with $\bar{e} = \frac{1}{n} \sum_{i=1}^n e_i$. Only the first p eigenvalues and eigenfunctions are retained, where $p = p(n)$ is a given integer, smaller than n .

3. Estimate $f(x/y)$ by

$$\hat{f}(x/y) = \exp \left\{ \sum_{j=1}^p \frac{\hat{\mu}_j(y)}{\hat{\lambda}_j} \left(\hat{x}_j - \frac{\hat{\mu}_j(y)}{2} \right) \right\}, \quad (5)$$

where $\hat{\mu}_j(y) = \langle \hat{\mu}(y), \hat{\varphi}_j \rangle$ and $\hat{x}_j = \langle x, \hat{\varphi}_j \rangle$.

Finally, substituting (5) into (3) leads to an estimate $\hat{\gamma}(x)$ of $\gamma(x)$, which will be referred to as the DBIR estimator. It can be proved that this estimator is consistent ($\lim_{n \rightarrow \infty} \hat{\gamma}(x) \stackrel{\mathbb{P}}{=} \gamma(x)$) under mild regularity assumptions.

3 A simulation study

In this section, the feasibility and the performances of the nonparametric functional regression method described in Section 2 is discussed through a simulation study.

3.1 Data generation

The data were simulated in the following way: values for the real random variable Y were drawn from a uniform distribution in the interval $[0, 10]$. Then, X was generated by 2 different models or settings:

M1 $X = Ye_1 + 2Ye_2 + 3Ye_5 + 4Ye_{10} + \epsilon,$

M2 $X = \sin(Y)e_1 + \log(Y + 1)e_5 + \epsilon,$

where $(e_i)_{i \geq 1}$ is the trigonometric basis of $\mathcal{X} = \mathcal{L}^2([0, 1])$ (i.e., $e_{2k-1} = \sqrt{2} \cos(2\pi kt)$, and $e_{2k} = \sqrt{2} \sin(2\pi kt)$), and ϵ a Gaussian process independent of Y with zero mean and covariance operator $\Gamma_e = \sum_{j \geq 1} \frac{1}{j} e_j \otimes e_j$. More precisely, ϵ was simulated by using a truncation of Γ_e , $\Gamma_e(s, t) \simeq \sum_{j=1}^q \frac{1}{j} e_j(t) e_j(s)$ by setting $q = 500$. From these two designs, training and a test samples were simulated with respective sizes $n_L = 300$ and $n_T = 200$.

Figures 1 and 2 give examples of realizations of X obtained under the first and the second model, respectively, for three different values of y . They also represent the underlying (non noisy) functions, $F(y)$. In the case of model **M2**, the simulated data have a high level of noise which makes the estimation a hard task.

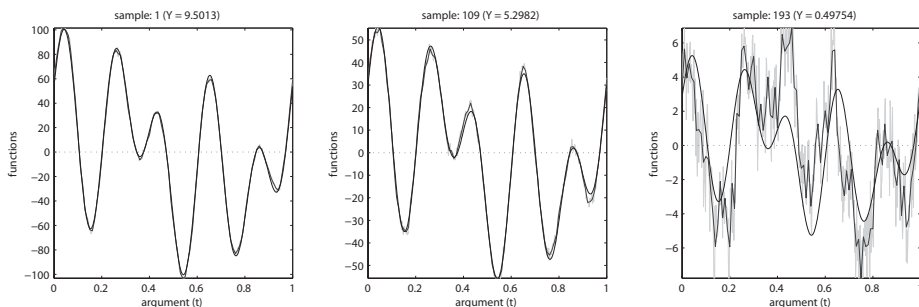


Figure 1: Model **M1**. True function $F(y)$ (smooth continuous line), simulated data X (gray rough line) and approximation of X using B-splines (rough black line) for three different values of y .

Finally, to apply the DBIR method, the discretized functions X were approximated by a continuous function using a functional basis expansion. Specifically, the data were approximated using 128 B-spline basis functions of order 4: Figures 1 and 2 show the comparison between the raw functions and their B-spline approximation.

3.2 Simulation results

The conditional mean $\mu(y)$ was estimated by a kernel smoothing (such as in Equation (4)). Two hyperparameters were to be tuned in this approach: the

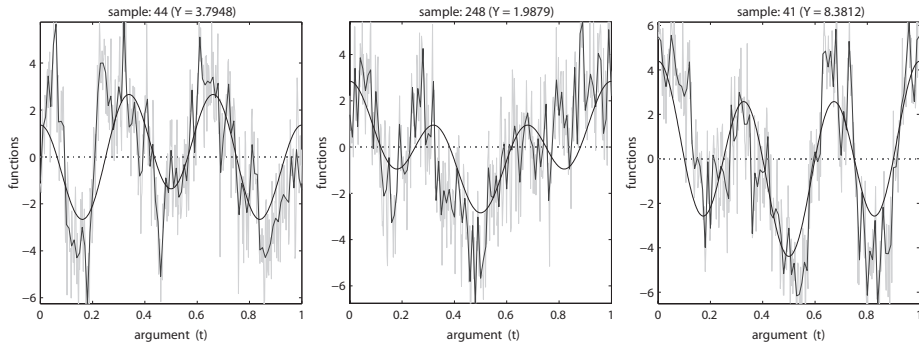


Figure 2: Model **M2**. True function $F(y)$ (smooth continuous line), simulated data X (gray rough line) and approximation of X using B-splines (rough black line) for three different values of y .

bandwidth parameter for the estimation of $\mu(y)$ and the number, p , of eigenfunctions involved in Equation (5). These two parameters were selected by a 10-fold cross-validation minimizing the mean square error (MSE) criterion on the training sampling.

3.2.1 Linear case: M1

This section gives the results obtained in the first simulated model, which presents a linear relation between the real explanatory variable and functional response variables in the inverse model of Equation (1). From Figure 1, it can be notice that the level of noise in the data is greater for small values of Y .

The estimation of the conditional mean using a kernel estimator (Equation (4)) is shown in Figure 3. A comparison between true values and estimated values of $F(y)(t)$ are given for various values of y (top) and for various values of t (bottom). The linearity of the inverse model of Equation (1) is illustrated by the linear $F(y)$ in the bottom part of this figure. In general, the estimates are good but, in some cases (e.g., bottom right) the level of noise appears to be too high and the true mean (as a function of y) it is not as well estimated as in the other cases.

Figure 4 shows the estimated eigendecomposition of the empirical covariance of residuals r (Section 2.2, step 2) and the predicted values of Y on the training and test sets by using the DBIR estimator. More specifically, the comparison between the true and the estimated eigenfunctions are shown in Figure 4 (a-c) and the comparison between the true and the estimated eigenvalues in Figure 4 (d). The results show very good predictions in both the training and test sets (Figure 4 (e-f)).

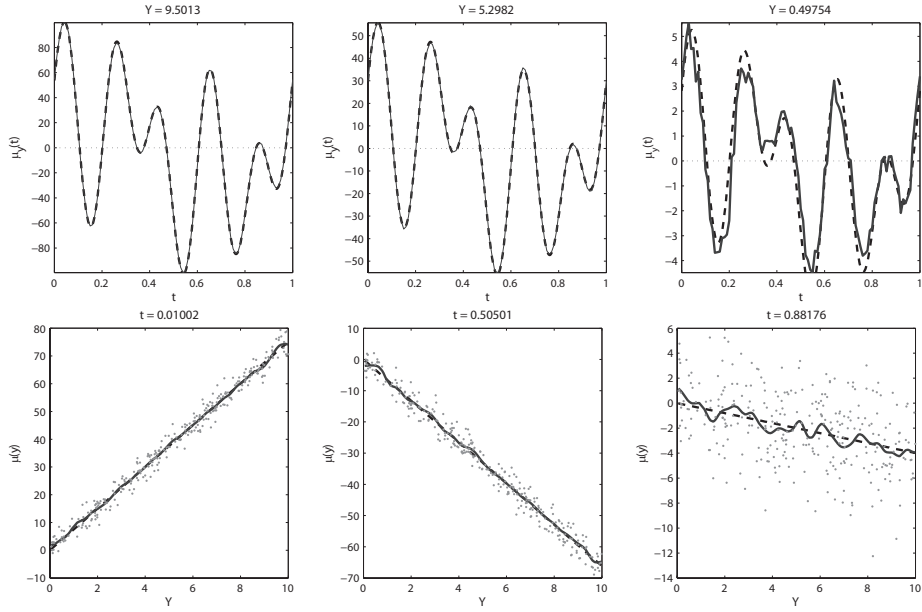


Figure 3: Model **M1**. Top: True values (discontinuous lines) and estimates (continuous lines) of $F(y)$ for various values of y . Bottom: true values and estimates of $F(\cdot)(t)$ for various values of t (bottom). The dots (bottom) are the simulated data $(x_i(t))_i$ in the training set.

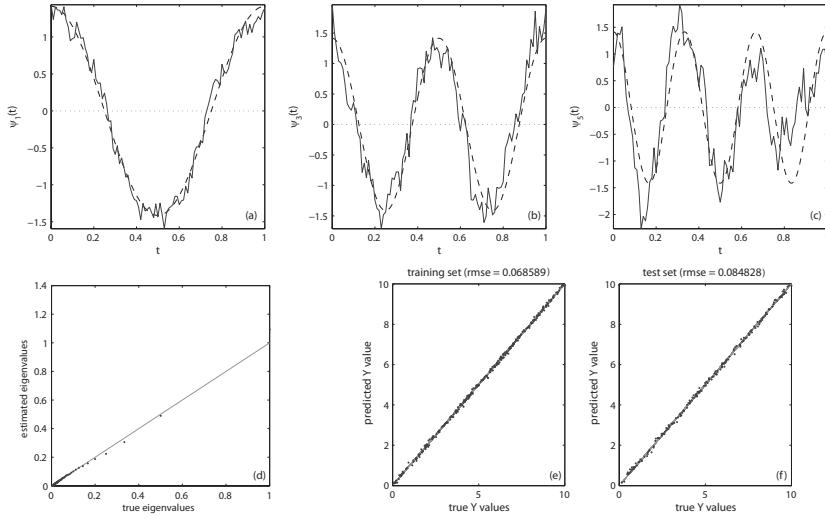


Figure 4: Model **M1**. (a-c): True (dashed line) and estimated eigenfunctions (continuous line); (d): estimated vs. true eigenvalues and (e-f): predicted values for Y vs. the true ones for training and test sets.

3.2.2 Nonlinear case: M2

For this nonlinear model **M2**, Figure 2 shows that the level of noise is much higher than for **M1**. In the same way as in the previous section, Figure 5 compares the true $F(y)(t)$ to its estimated values for various values of y (top) and for various values of t (bottom). The results are very satisfactory given the fact that the data have a high level of noise (which clearly appears in the bottom of this figure).

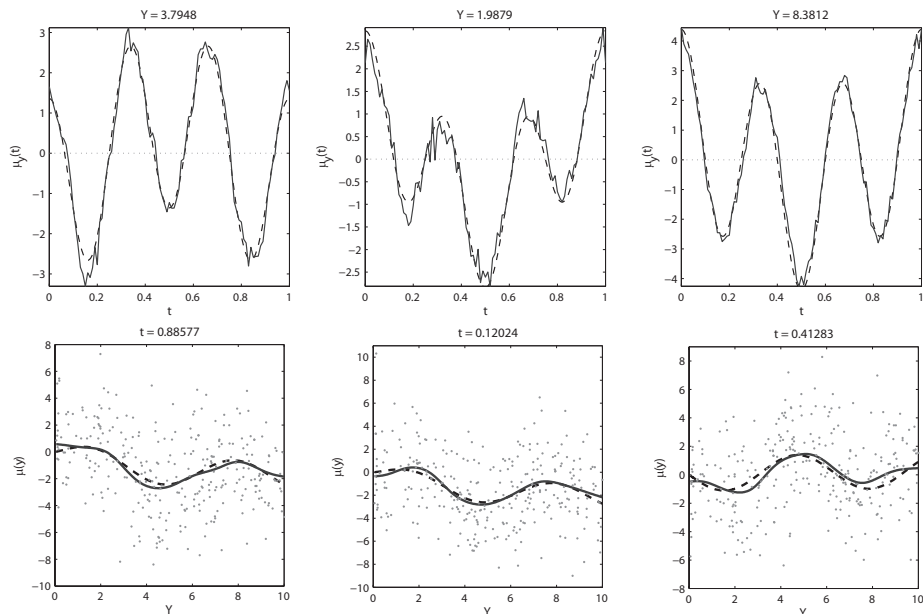


Figure 5: Model **M2**. Top: True values (discontinuous lines) and estimates (continuous lines) of $F(y)$ for various values of y . Bottom: true values and estimates of $F(\cdot)(t)$ for various values of t (bottom). The dots (bottom) are the simulated data $(x_i(t))_i$ in the training set.

Figure 6 shows the results of the steps 2-3 of the estimation scheme: the estimated eigendecomposition of r is compared to the true one, and the predicted value for Y are compared to the true ones, both on training and test sets. The estimation of the eigendecomposition is also very satisfactory despite the high level of noise, and the comparison between training and test sets shows that the method does not overfit the data.

4 Conclusion

A new functional nonparametric regression approach has been introduced motivated by the calibration problems in Chemometrics. The new method, named

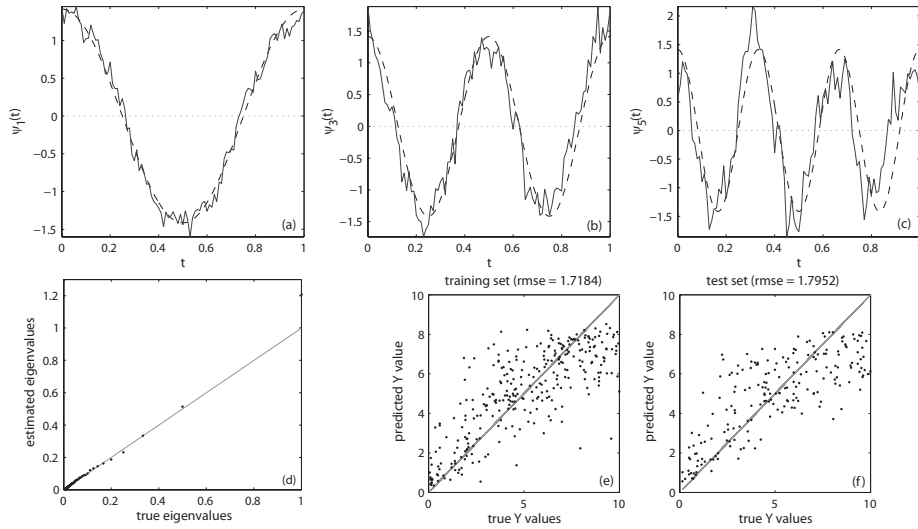


Figure 6: Model **M2**: (a-c): True (dashed line) and estimated eigenfunctions (continuous line); (d): estimated vs. true eigenvalues and (e-f): predicted values for Y vs. the true ones for training and test sets.

functional Density-Based Inverse Regression (DBIR) was fully described for the sample space $\mathcal{X} = L_2([a, b])$ under a Gaussian assumption for the conditional law $P(\cdot|Y)$ but it can be extended to other sample spaces and distribution families. Two appealing features of the new method are its rather mild model assumptions and its computational simplicity. The simulation study of DBIR has shown that it performs well for both linear and nonlinear models. Thus, DBIR can be considered as a promising functional regression methods, particularly appealing for calibration problems.

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