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Smoothing Splines Estimators in Functional Linear Regression with Errors-in-Variables

by

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Smoothing Splines Estimators in Functional Linear Regression with Errors-in-Variables

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Abstract This work deals with a generalization of the Total Least Squares method in the context of the functional linear model. We first propose a smoothing splines estimator of the functional coefficient of the model without noise in the covariates and we obtain an asymptotic result for this estimator. Then, we adapt this estimator to the case where the covariates are noisy and we also derive an upper bound for the convergence speed. Our estimation procedure is evaluated by means of simulations.

Key words Functional Linear Model, Smoothing Splines, Penalization, Errors-in-Variables, Total Least Squares.

1 Introduction

A very common problem in statistics is to explain the effects of a covariate X on a random variable Y (variable of interest), defined on a probability space (Ω, \mathcal{A}, P) . We consider here a real variable Y , while X is supposed to belong to some separable Hilbert space H , endowed with an inner product noted $\langle \cdot, \cdot \rangle$. The model we consider here is a linear model in the sense that we write

$$Y = \langle \alpha, X \rangle + \epsilon, \quad (1)$$

where $\alpha \in H$ is unknown and ϵ is a real random variable satisfying $\mathbb{E}(\epsilon) = 0$ and $\mathbb{E}(\epsilon^2) = \sigma_\epsilon^2$. Considering data $(X_i, Y_i)_{i=1, \dots, n}$, the goal is then to estimate

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$\alpha \in H$. Let us notice here that there can be different ways to generate the curves X_i . One possibility is a fixed design, that is, X_1, \dots, X_n are fixed, non-random functions. Examples are experiments in chemical or engineering applications, where X_i corresponds to functional responses obtained under various, predetermined experimental conditions (see for instance [6]). In other applications one may assume a random design, where X_1, \dots, X_n are an i.i.d. sample of H . In any case, Y_1, \dots, Y_n are independent and the expectations above always refer to the probability distribution induced by the random variable ϵ , only. In the case of random design, they thus formally have to be interpreted as conditional expectation given X_1, \dots, X_n .

However, if we have a closer look at this model (1), we can remark that there is the underlying assumption that X is observed without error, and all the errors are confined to the variable Y by the way of ϵ . Unfortunately, this assumption does not seem to be very realistic in practice, and many errors (modeling errors, instrument errors, human errors, ...) prevent to know X_1, \dots, X_n exactly. That is why we naturally consider the fact that X is not directly observed, but the available variable is actually

$$W = X + \delta, \quad (2)$$

where δ is a noise random variable. This problem of the *Errors-in-Variables* linear model has already been studied in many ways in the case where H is \mathbb{R} or \mathbb{R}^p , that is to say when X is an univariate or a multivariate predictor. For instance, the maximum likelihood method has been applied to this context (see [11]), and asymptotic results have been obtained (see for example [14]). Because this problem is strongly linked to the problem of solving linear systems

$$\mathbf{A}\mathbf{x} \approx \mathbf{b},$$

where $\mathbf{x} \in \mathbb{R}^p$ is unknown, $\mathbf{b} \in \mathbb{R}^n$ and \mathbf{A} is a matrix of size $n \times p$, some numerical approaches have also been proposed. One of the most famous is the *Total Least Squares* (TLS) method (see for example [16] or [26]).

In many applications (for instance in climatology, teledetection, linguistics, ...), the data come from the observation of continuous phenomenons of time or space. Due to important performances of measurement instruments, the collected data can be seen as curves or surfaces, and cannot be considered anymore as variables taking values in \mathbb{R}^p . They are variables taking values in some functional Hilbert space H . These so-called *functional data* have been studied a lot these last years (to get a theoretical and practical overview on functional data, we refer to the books [1], [21], [22] and [10]).

In this paper, our goal is to study a way to deal with the *Errors-in-Variables* linear model in the context where the covariate X is of functional nature. In what follows, we consider that H is the space $L^2(I)$ of functions $f : I \rightarrow \mathbb{R}$ defined on an interval I of \mathbb{R} such that $\int_I f(t)^2 dt$ is finite. This space is endowed with its usual inner product $\langle \cdot, \cdot \rangle$ defined by $\langle f, g \rangle = \int_I f(t)g(t)dt$ for $f, g \in L^2(I)$, and the associated norm is noted $\|\cdot\|_{L^2}$. In order to simplify expressions, we take $I = [0, 1]$ all along the paper. Now, in this context, the model (1) can be written as in [20]

$$Y = \int_I \alpha(t)X(t)dt + \epsilon, \quad (3)$$

where $\alpha \in L^2(I)$ is unknown and has to be estimated using the sample $(W_i, Y_i)_{i=1, \dots, n}$ with W_1, \dots, W_n noisy observations of X_1, \dots, X_n . In practice, the whole curves are not available, so we suppose in the following that the curves are observed in p discretization points $t_1 < \dots < t_p$ belonging to I , that we will take equispaced in order to simplify, such that $t_j - t_{j-1} = \frac{1}{p}$ for all $j = 2, \dots, p$. The discretized version of the inner product $\langle \cdot, \cdot \rangle$ will be denoted by $\langle \cdot, \cdot \rangle_p$ and defined for $f, g \in L^2(I)$ by

$$\langle f, g \rangle_p = \frac{1}{p} \sum_{j=1}^p f(t_j)g(t_j).$$

This approximation of $\langle \cdot, \cdot \rangle$ by $\langle \cdot, \cdot \rangle_p$ is valid only if p is large enough, so we assume this from now on. In this context of discretized curves, relations (2) and (3) then write

$$Y = \frac{1}{p} \sum_{j=1}^p \alpha(t_j)X(t_j) + \epsilon, \quad (4)$$

and, for $j = 1, \dots, p$

$$W(t_j) = X(t_j) + \delta(t_j), \quad (5)$$

where $(\delta(t_j))_{j=1, \dots, p}$ is a sequence of independent real random variables, such that, for all $j = 1, \dots, p$

$$\mathbb{E}(\delta(t_j)) = 0,$$

and

$$\mathbb{E}(\delta(t_j)^2) = \sigma_\delta^2.$$

It is worth noting that, when there is no error on the variable X , many practical and theoretical works have been performed concerning the estimation of the functional coefficient α using a sample $(X_i, Y_i)_{i=1, \dots, n}$ (see for instance [6] in the case of a functional response, and also [3], [4] and references therein for the case of a random covariate X). We choose here another way to estimate α , using an approach derived from smoothing splines (see [9] for an overview on smoothing splines).

The paper is organized as follows. In section 2, we present the smoothing splines estimation procedure and the convergence result for this estimator in the case where the covariate X is non-noisy. In section 3, we present the generalization of the *TLS* method to the case where X is a functional random variable and we give a convergence result for the estimator introduced in section 2. We make some comments about these results in section 4. Section 5 is devoted to some numerical simulations presenting an evaluation of our estimation procedure. Finally, in section 6, we give the proof of our results.

2 Estimation of α in the non-noisy case

From now on, we adopt the following matrix notations: $\mathbf{Y} = (Y_1, \dots, Y_n)^\tau$, $\mathbf{X}_i = (X_i(t_1), \dots, X_i(t_p))^\tau$ for all $i = 1, \dots, n$, $\boldsymbol{\alpha} = (\alpha(t_1), \dots, \alpha(t_p))^\tau$ and $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_n)^\tau$. Moreover, we denote by \mathbf{X} the $n \times p$ matrix with general term $X_i(t_j)$ for all $i = 1, \dots, n$ and for all $j = 1, \dots, p$. Using these notations, the model (4) then writes

$$\mathbf{Y} = \frac{1}{p} \mathbf{X} \boldsymbol{\alpha} + \boldsymbol{\epsilon}. \quad (6)$$

We want to estimate $\boldsymbol{\alpha}$ as the values of a smooth function at the measurement points, so we assume that α is m times differentiable (with $m \in \mathbb{N}$).

Our estimation procedure is motivated by the usual smoothing splines approach in nonparametric regression. For some noisy observations z_i of a smooth function $f(t_i)$ at design points t_1, \dots, t_p , an estimate \hat{f} is obtained by minimizing $\frac{1}{p} \sum_i (z_i - v(t_i))^2 + \rho \int_I v^{(m)}(t)^2 dt$ for some smoothing parameter $\rho > 0$. Minimization takes place over all functions v in an m -th order Sobolev space, that is $D^m v \in L^2(I)$. It can be shown (for an overview of results in spline theory, consider [7] and [9]) that the solution \hat{f} is in the space $NS^m(t_1, \dots, t_p)$ of *natural splines* of order $2m$ with knots at t_1, \dots, t_p . This is a p -dimensional linear functions space with $D^m v \in L^2(I)$ for any $v \in NS^m(t_1, \dots, t_p)$, and there exist basis functions b_1, \dots, b_p such that $NS^m(t_1, \dots, t_p) = \left\{ \sum_j \theta_j b_j \mid \theta_1, \dots, \theta_p \in \mathbb{R} \right\}$. Different possible basis

functions proposed by various authors are discussed in [9]. For any vector $\mathbf{w} = (w_1, \dots, w_p)^\tau \in \mathbb{R}^p$, there exists a unique natural spline interpolant $s_{\mathbf{w}}$ with $s_{\mathbf{w}}(t_j) = w_j$, $j = 1, \dots, p$. With $\mathbf{b}(t) = (b_1(t), \dots, b_p(t))^\tau$ and \mathbf{B} denoting the $p \times p$ matrix with elements $b_i(t_j)$, $s_{\mathbf{w}}$ is given by

$$s_{\mathbf{w}}(t) = \mathbf{b}(t)^\tau (\mathbf{B}^\tau \mathbf{B})^{-1} \mathbf{B}^\tau \mathbf{w}. \quad (7)$$

The important property of such a spline interpolant is the fact that

$$\begin{aligned} \int_I s_{\mathbf{w}}^{(m)}(t)^2 dt &\leq \int_I f^{(m)}(t)^2 dt \text{ for any other function } f \\ \text{with } f^{(m)} &\in L^2(I) \text{ and } f(t_j) = w_j, j = 1, \dots, p. \end{aligned} \quad (8)$$

When considering the above minimization problem, (8) implies that the solution \hat{f} is given by $\hat{f} = s_{\hat{\mathbf{w}}}$, where $\hat{\mathbf{w}}$ is obtained by minimizing $\frac{1}{p} \sum_i (z_i - w_i)^2 + \rho \int_I s_{\mathbf{w}}^{(m)}(t)^2 dt$ over all vectors $\mathbf{w} \in \mathbb{R}^p$.

These ideas readily generalize to the problem of estimating α in (6). An estimator $\hat{\alpha}_{FLS,X}^*$ may be obtained by solving the minimization problem

$$\min_{\mathbf{a} \in \mathbb{R}^p} \left\{ \frac{1}{n} \left\| \mathbf{Y} - \frac{1}{p} \mathbf{X} \mathbf{a} \right\|^2 + \rho \int_I s_{\mathbf{a}}^{(m)}(t)^2 dt \right\}, \quad (9)$$

where $\|\cdot\|$ stands for the usual Euclidean norm, and $\rho > 0$ is a smoothing parameter allowing a trade-off between the goodness-of-fit to the data and the smoothness of the fit. Then, $\hat{\alpha} = s_{\hat{\alpha}_{FLS,X}^*}$ provides a corresponding estimate of the function α . By (7), we have $\int_I s_{\mathbf{a}}^{(m)}(t)^2 dt = \mathbf{a}^\tau \mathbf{A}_m^* \mathbf{a}$, where $\mathbf{A}_m^* = \mathbf{B} (\mathbf{B}^\tau \mathbf{B})^{-1} [\int_I \mathbf{b}^{(m)}(t) \mathbf{b}^{(m)}(t)^\tau dt] (\mathbf{B}^\tau \mathbf{B})^{-1} \mathbf{B}^\tau$ is a $p \times p$ matrix. Therefore, (9) can be reformulated in the form

$$\min_{\mathbf{a} \in \mathbb{R}^p} \left\{ \frac{1}{n} \left\| \mathbf{Y} - \frac{1}{p} \mathbf{X} \mathbf{a} \right\|^2 + \rho \mathbf{a}^\tau \mathbf{A}_m^* \mathbf{a} \right\}, \quad (10)$$

leading to the solution

$$\hat{\alpha}_{FLS,X}^* = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \rho \mathbf{A}_m^* \right)^{-1} \mathbf{X}^\tau \mathbf{Y} = \frac{1}{n} \left(\frac{1}{np} \mathbf{X}^\tau \mathbf{X} + \rho p \mathbf{A}_m^* \right)^{-1} \mathbf{X}^\tau \mathbf{Y}.$$

However, there is a problem with this estimator which is due to the structure of the eigenvalues of $p \mathbf{A}_m^*$. These eigenvalues have been studied by many authors, a discussion of general results is given by [9]. The most precise results in our context are presented in [25]. It is shown that this

matrix has exactly m zero eigenvalues $\mu_{1,p} = \dots = \mu_{m,p} = 0$, while as $p \rightarrow \infty$,

$$\sum_{j=m+1}^p \frac{1}{\mu_{j,p}} \rightarrow \sum_{j=m+1}^{\infty} (\pi j)^{-2m}, \quad (11)$$

where $0 < \mu_{m+1,p} < \dots < \mu_{p,p}$ denote the $p - m$ non-zero eigenvalues of $p\mathbf{A}_m^*$. The series given in (11) converges for $m \neq 0$, so we assume this in the following.

Due to the m zero eigenvalues, existence of $\hat{\boldsymbol{\alpha}}_{FLS,X}^*$ can only be guaranteed by introducing constraints on the structure of \mathbf{X} . This can, however, be avoided by introducing a minor modification of this estimator. The m -dimensional eigenspace corresponding to $\mu_{1,p} = \dots = \mu_{m,p} = 0$ is the linear vector space generated by all (discretized) polynomials of degree m , that is, E_m consists of all vectors $\mathbf{w} \in \mathbb{R}^p$ with $w_i = \theta_1 + \sum_{j=1}^m \theta_{j+1} t_i^j$, $i = 1, \dots, p$, for some coefficients $\theta_1, \dots, \theta_{m+1}$. Let \mathbf{P}_m denote the $p \times p$ projection matrix projecting into the space E_m , and set $\mathbf{A}_m = \mathbf{P}_m + p\mathbf{A}_m^*$. Our final estimator $\hat{\boldsymbol{\alpha}}_{FLS,X}$ is then defined by

$$\hat{\boldsymbol{\alpha}}_{FLS,X} = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{X}^T \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \mathbf{X}^T \mathbf{Y} = \frac{1}{n} \left(\frac{1}{np} \mathbf{X}^T \mathbf{X} + \rho \mathbf{A}_m \right)^{-1} \mathbf{X}^T \mathbf{Y}. \quad (12)$$

It is immediately verified that $\hat{\boldsymbol{\alpha}}_{FLS,X}$ is solution of the modified minimization problem

$$\min_{\mathbf{a} \in \mathbb{R}^p} \left\{ \frac{1}{n} \left\| \mathbf{Y} - \frac{1}{p} \mathbf{X} \mathbf{a} \right\|^2 + \frac{\rho}{p} \mathbf{a}^T \mathbf{A}_m \mathbf{a} \right\}.$$

By definition, the matrix \mathbf{A}_m possesses m eigenvalues equal to 1, while the remaining $p - m$ eigenvalues coincide with the eigenvalues $\mu_{m+1,p} < \dots < \mu_{p,p}$ of $p\mathbf{A}_m^*$. Thus, by (11), we obtain $\text{Tr}(\mathbf{A}_m^{-1}) \rightarrow \sum_{j=m+1}^{\infty} (\pi j)^{-2m} + m =: C_0$ as $p \rightarrow \infty$. It follows that for any constant $C_1 > C_0$ there exists a $p_0 \in \mathbb{N}$ such that

$$\text{Tr}(\mathbf{A}_m^{-1}) \leq C_1, \quad (13)$$

for all $p \geq p_0$.

We will now study the behavior of our estimator for large values of n and p . In addition to the usual Euclidean norm bias of our estimator will be evaluated with respect to the semi-norm

$$\|\mathbf{u}\|_{\Gamma}^2 = \frac{1}{p} \mathbf{u}^T \left(\frac{1}{np} \mathbf{X}^T \mathbf{X} \right) \mathbf{u}.$$

It is well-known that functional linear regression belongs to the class of ill-posed problems. The above semi-norm may be seen as a discretized version of L^2 semi-norms which are usually applied in this context. It is not possible to derive any bound for the bias by using the Euclidean norm. Suppose, for example, that all functions X_i lie in a low dimensional linear function space \mathcal{X} . Then any structure of α which is orthogonal to \mathcal{X} cannot be identified from the data.

We will need in the following the additional assumption:

(H.1) α is m times differentiable and $\alpha^{(m)}$ belongs to $L^2(I)$.

Then, let $C_2 = \int_I \alpha^{(m)}(t)^2 dt$ and $C_3^* = \int_I \alpha(t)^2 dt$. By construction of \mathbf{P}_m , $\mathbf{P}_m \mathbf{a}$ provides the best approximation (in a least squares sense) of \mathbf{a} by (discretized) polynomials of degree m , and $\frac{1}{p} \mathbf{a}^T \mathbf{P}_m \mathbf{a} \leq \frac{1}{p} \mathbf{a}^T \mathbf{A}_m \mathbf{a} \rightarrow C_3^*$ as $p \rightarrow \infty$. Let C_3 denote an arbitrary constant with $C_3^* < C_3 < \infty$. There then exists a $p_1 \in \mathbb{N}$ with $p_1 \geq p_0$ such that $\frac{1}{p} \mathbf{a}^T \mathbf{P}_m \mathbf{a} \leq C_3$ for all $p \geq p_1$.

As noticed before, X_1, \dots, X_n can be either fixed, non-random functions or an i.i.d. sample of random functions. In any case, expected values and variance of $\hat{\alpha}_{FLS,X}$ as stated in the theorem will refer to the probability distribution induced by the random variable ϵ . In the case of random design, they stand for conditional expectation given X_1, \dots, X_n .

Theorem 1 *Under hypothesis (H.1) and the above definitions of C_1 , C_2 , C_3 , p_1 , we obtain for all $n \in \mathbb{N}$, all $p \geq p_1$ and every matrix $\mathbf{X} \in \mathbb{R}^n \times \mathbb{R}^p$*

$$\|\mathbb{E}(\hat{\alpha}_{FLS,X}) - \alpha\|_{\Gamma}^2 \leq \rho \left(\frac{1}{p} \mathbf{a}^T \mathbf{P}_m \mathbf{a} + C_2 \right) \leq \rho (C_3 + C_2), \quad (14)$$

as well as

$$\frac{1}{p} \mathbb{E} (\|\hat{\alpha}_{FLS,X} - \mathbb{E}(\hat{\alpha}_{FLS,X})\|^2) \leq \frac{\sigma_{\epsilon}^2}{n\rho} C_1. \quad (15)$$

Remark

When adding some additional constraint like

(H.2) $\sup_i \sup_j |X_i(t_j)| \leq C_4 < +\infty$ (or $P(\sup_i \sup_j |X_i(t_j)| \leq C_4) = 1$ in the case of a random design) for all n, p ,

then the variance can also bound the above semi-norm,

$$\|\hat{\alpha}_{FLS,X} - \mathbb{E}(\hat{\alpha}_{FLS,X})\|_{\Gamma}^2 \leq \frac{C_4}{p} \mathbb{E} (\|\hat{\alpha}_{FLS,X} - \mathbb{E}(\hat{\alpha}_{FLS,X})\|^2),$$

and the theorem implies that

$$\|\hat{\alpha}_{FLS,X} - \alpha\|_{\Gamma}^2 = O_P \left(n^{-1/2} \right),$$

if $\rho \sim n^{-1/2}$ as $n \rightarrow \infty$. This rate obviously compares favorably to existing rates in the literature.

3 Total Least Squares method for functional covariates

In this section, we present the *TLS* method when the noisy covariate X is of functional nature. At first, let us describe how things work in the case of a covariate \mathbf{X} belonging to \mathbb{R} or \mathbb{R}^p . In that case, considering a sample, equations (1) and (2) then write, for $i = 1, \dots, n$

$$Y_i = \mathbf{X}_i^\tau \boldsymbol{\alpha} + \epsilon_i,$$

with $\boldsymbol{\alpha}$ and $\mathbf{X}_1, \dots, \mathbf{X}_n$ belonging to \mathbb{R}^p , and

$$\mathbf{W}_i = \mathbf{X}_i + \boldsymbol{\delta}_i,$$

with $\mathbf{W}_i = (W_{i1}, \dots, W_{ip})^\tau$ and $\boldsymbol{\delta}_i$ belonging to \mathbb{R}^p for all $i = 1, \dots, n$. This leads us (see for example [26]) to determine simultaneously $\boldsymbol{\alpha}$ and \mathbf{X}_i by considering the minimization problem

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^p, \mathbf{X}_i \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \left[(Y_i - \mathbf{X}_i^\tau \boldsymbol{\alpha})^2 + (\mathbf{X}_i - \mathbf{W}_i)^\tau (\mathbf{X}_i - \mathbf{W}_i) \right] \right\}. \quad (16)$$

The *TLS* algorithm solving (16) is given in [26]. In some cases, the singular values of the matrix \mathbf{W} can quickly decrease to zero, and the minimization problem (16) is then *ill-conditioned*. A possible way to circumvent this problem is to introduce a regularization in (16), and the minimization problem we consider is then (see [15])

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^p, \mathbf{X}_i \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \left[(Y_i - \mathbf{X}_i^\tau \boldsymbol{\alpha})^2 + (\mathbf{X}_i - \mathbf{W}_i)^\tau (\mathbf{X}_i - \mathbf{W}_i) \right] + \rho \boldsymbol{\alpha}^\tau \mathbf{L}^\tau \mathbf{L} \boldsymbol{\alpha} \right\}, \quad (17)$$

where \mathbf{L} is a $p \times p$ matrix and ρ is a regularization parameter allowing to deal with the ill-conditioning of the design matrix $\mathbf{W}^\tau \mathbf{W}$. Indeed, the *TLS* solution to the minimization problem (17) is given by

$$\hat{\boldsymbol{\alpha}}_{TLS} = (\mathbf{W}^\tau \mathbf{W} + \rho \mathbf{L}^\tau \mathbf{L} - \sigma_k^2 \mathbf{I}_p)^{-1} \mathbf{W}^\tau \mathbf{Y}, \quad (18)$$

where σ_k is the smallest non-zero singular value of the matrix (\mathbf{W}, \mathbf{Y}) and \mathbf{I}_p is the $p \times p$ identity matrix.

In our functional situation, considering a sample and using the same matricial notations as in section 2, the model considered then writes

$$\mathbf{Y} = \frac{1}{p} \mathbf{X} \boldsymbol{\alpha} + \boldsymbol{\epsilon},$$

and

$$\mathbf{W} = \mathbf{X} + \boldsymbol{\delta},$$

where \mathbf{W} and $\boldsymbol{\delta}$ are the $n \times p$ matrices with respective general terms $W_i(t_j)$ and $\delta_i(t_j)$. So, the minimization problem that we consider now is the following one: we are looking for an estimation $\hat{\boldsymbol{\alpha}}_{FTLS}$ of $\boldsymbol{\alpha}$, solution of the minimization problem

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^p, \mathbf{X}_i \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \left[\left(Y_i - \frac{1}{p} \mathbf{X}_i^T \boldsymbol{\alpha} \right)^2 + \frac{1}{p} \|\mathbf{X}_i - \mathbf{W}_i\|^2 \right] + \frac{\rho}{p} \boldsymbol{\alpha}^T \mathbf{A}_m \boldsymbol{\alpha} \right\}, \quad (19)$$

where the matrix \mathbf{A}_m is the one introduced in section 2. Now, with these notations, we have the following result.

Proposition 1 *The solution of the minimization problem (19) is given by*

$$\hat{\boldsymbol{\alpha}}_{FTLS} = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{W}^T \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \sigma_k^2 \mathbf{I}_p \right)^{-1} \mathbf{W}^T \mathbf{Y}, \quad (20)$$

where σ_k^2 is the smallest non-zero eigenvalue of the matrix

$$\frac{1}{n} \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right)^T \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right) + \frac{\rho}{p} \begin{pmatrix} \mathbf{A}_m & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix}.$$

In equation (20), computational problems can appear due to the value of σ_k^2 . Indeed, the eigenvalues of $\frac{1}{n} \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right)^T \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right)$ are known to decrease rapidly to zero, and this can of course cause numerical problems with the computation of σ_k^2 . Nevertheless, we can circumvent this problem using the following result.

Proposition 2 *Let us consider the following hypothesis:*

(H.3) *There exists a constant $C_5 > 0$ such that*

$$\sup_{r,s=1,\dots,p} \mathbb{E} (\delta_i(t_r)^2 \delta_i(t_s)^2) \leq C_5.$$

Then, under (H.2) and (H.3), we have

$$\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} = \frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\sigma_\delta^2}{p^2} \mathbf{I}_p + \mathbf{R}, \quad (21)$$

where \mathbf{R} is a matrix such that $\|\mathbf{R}\| = O_P\left(\frac{1}{n^{1/2}p}\right)$, $\|\cdot\|$ being the usual norm of a matrix.

The last problem is that σ_δ^2 is not always known. There are several ways to estimate it. We choose to use the estimator presented in [13] and given by (as we are in the case of equispaced measurement points)

$$\hat{\sigma}_\delta^2 = \frac{1}{n} \sum_{i=1}^n \frac{1}{6(p-2)} \sum_{j=2}^{p-1} [W_i(t_{j-1}) - W_i(t_j) + W_i(t_{j+1}) - W_i(t_j)]^2. \quad (22)$$

This leads us to change the former estimator of α given by (20) and to take instead

$$\hat{\alpha}_{FTLS} = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \frac{\hat{\sigma}_\delta^2}{p^2} \mathbf{I}_p \right)^{-1} \mathbf{W}^\tau \mathbf{Y}. \quad (23)$$

The asymptotic behavior of this estimator is given by the following theorem.

Theorem 2 *Under hypotheses (H.1) - (H.3), if we also assume that $Y_i \perp\!\!\!\perp \delta_i$ for all $i = 1, \dots, n$ and that $\mathbb{E}(Y_i^2) < +\infty$, then we have*

$$\|\hat{\alpha}_{FTLS} - \hat{\alpha}_{FLS,X}\| = O_P\left(\frac{\sigma_\delta}{n^{1/2}p^{1/2}\rho}\right). \quad (24)$$

4 Some comments

(i) In the expression (23) of the estimator of α , the term $-\frac{\hat{\sigma}_\delta^2}{p^2} \mathbf{I}_p$ acts as a deregularization term. It allows us to deal with the bias introduced by the fact that we only know the matrix \mathbf{W} instead of the “true” one \mathbf{X} .

(ii) In theorem 2, the order $\sigma_\delta/(n^{1/2}p^{1/2}\rho)$ given by relation (24) is a result in accordance with the intuition. The estimation will be improved for a high number p of discretization points and will collapse (at least in practice, see the simulations in section 5) if σ_δ becomes too high.

(iii) An immediate corollary of theorems 1 and 2 is

$$\|\hat{\alpha}_{FTLS} - \alpha\|_\Gamma^2 = O_P\left(\frac{1}{n\rho} + \rho + \frac{\sigma_\delta^2}{np\rho^2}\right).$$

If we compare these three terms, we can see that, for p large enough (more precisely for p such that $p\rho$ goes to infinity as n goes to infinity), it remains

$$\|\hat{\alpha}_{FTLS} - \alpha\|_{\Gamma}^2 = O_P\left(\frac{1}{n\rho} + \rho\right),$$

and then, for $\rho \sim n^{-1/2}$,

$$\|\hat{\alpha}_{FTLS} - \alpha\|_{\Gamma}^2 = O_P\left(n^{-1/2}\right).$$

This means that, if the number of discretization points is large enough, we obtain the same upper bound for the convergence speed of the *FTLS* estimator as the *FLS* estimator using the true curves X_1, \dots, X_n . On the other hand, when p goes slowly to infinity (more precisely if $1/p$ goes to zero slower than ρ), then the contribution of the term $\sigma_{\delta}^2/(np\rho^2)$ may not be negligible anymore. In that case, if we still take $\rho \sim n^{-1/2}$, then we will have $\|\hat{\alpha}_{FTLS} - \alpha\|_{\Gamma}^2 = O_P(1/p) = O_P(n^{-\gamma})$ with $0 < \gamma < 1/2$.

(iv) Let us see what happens for the *FLS* estimator using the noisy curves W_1, \dots, W_n . The estimator of α is then given by

$$\hat{\alpha}_{FLS,W} = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{W}^T \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \mathbf{W}^T \mathbf{Y}. \quad (25)$$

If p is large enough, a calculus analogous to the one used in the proof of theorem 2 leads us to

$$\|\hat{\alpha}_{FLS,W} - \hat{\alpha}_{FLS,X}\| = O_P\left(\frac{\sigma_{\delta}}{n^{1/2}p^{1/2}\rho}\right),$$

that is to say we have the same upper bound of convergence speed for $\hat{\alpha}_{FLS,W}$ and $\hat{\alpha}_{FTLS}$. However, if p is not large enough (more precisely if p is negligible compared with $n^{1/2}$ and if $p\rho$ goes to zero as n goes to infinity), then we obtain

$$\|\hat{\alpha}_{FLS,W} - \hat{\alpha}_{FLS,X}\| = O_P\left(\frac{\sigma_{\delta}}{n^{1/2}p^{3/2}\rho^2}\right),$$

which is then an upper bound bigger than the previous one. However, these results are upper bounds and we do not know if we can do better. Nevertheless, the results obtained in the simulations (see section 5) allow us to think that we improve the estimation (see last remark) using the *FTLS* estimator instead of the *FLS* estimator with the noisy curves W_1, \dots, W_n .

(v) Using some heuristic arguments to expand the mean quadratic error of estimation of α (similarly to what is done in [2]), we can see that it is

generally better to consider the *FTLS* estimator compared to the *FLS* one with the variable W . More precisely, using the same notations as before, let us denote

$$\hat{\alpha}(\lambda) = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{W}^T \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \lambda \mathbf{I}_p \right)^{-1} \mathbf{W}^T \mathbf{Y},$$

where λ is a positive real number such that the matrix $\frac{1}{np^2} \mathbf{W}^T \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \lambda \mathbf{I}_p$ is positive definite. Then we have the following result, which proof is given in section 6.

Proposition 3 *Let $MISE(\lambda) = \mathbb{E}[(\hat{\alpha}(\lambda) - \alpha)^T (\hat{\alpha}(\lambda) - \alpha)]$. If we assume that $(\mathbf{W}^T \mathbf{W})^{-1}$ exists and if $\rho \|\mathbf{A}_m\|$ is negligible compared to $\left\| \frac{1}{np} \mathbf{W}^T \mathbf{W} \right\|$, then we have*

$$\frac{\partial}{\partial \lambda} MISE(\lambda)|_{\lambda=0} < 0.$$

In other words, this result means that it is advantageous to put a deregularization term $-\lambda \mathbf{I}_p$ (with a small positive λ) in order to improve the quality of the estimation relatively to the *MISE* criterion.

5 A simulation study

5.1 Presentation of the simulation

The aim of this simulation is to evaluate the performances of our estimator $\hat{\alpha}_{FTLS}$, and to compare it with $\hat{\alpha}_{FLS,W}$. We also compare $\hat{\alpha}_{FTLS}$ to $\hat{\alpha}_{FLS,\widetilde{W}}$, which is given by the same formula (25) except the fact that the curve W is replaced by a smoothed version \widetilde{W} . We can think that the smoothing has a correcting effect on the noisy curve W , then this smoothed curve \widetilde{W} can be expected to be closer than W from the unknown “true” curve X . This gives us the intuition that the estimator $\hat{\alpha}_{FLS,\widetilde{W}}$ should be better than $\hat{\alpha}_{FLS,W}$. To obtain a smoothed version \widetilde{W} of W , we choose to use the Nadaraya-Watson kernel estimator (see for example [18] or [23]). In the simulations, the kernel will be the standard normal kernel and the bandwidth will be chosen by cross validation (see [18]). In order to synthesize results, we only give the simulation results when X is non-random (when X is random, the simulation we have done lead to the same kind of conclusions). We have simulated $N = 100$ samples, each being composed of $n = 200$ observations $(W_i, Y_i)_{i=1,\dots,n}$ from the model given by (3) and (5), where the fixed design curves X_1, \dots, X_n are defined on $I = [0, 1]$ by

$$X_i(t) = \begin{cases} 10 \sin(2\pi it) & \text{if } i \text{ is even,} \\ 10 \cos(2\pi it) & \text{if } i \text{ is odd,} \end{cases}$$

similarly to what is used for the simulation in [6]. Each sample is randomly split into a learning sample of length $n_l = 100$ (this sample is used to build the estimator) and a test sample of length $n_t = 100$ (this sample is used to see the quality of the estimator by the way of computation of error terms). We make the simulations for different numbers of discretization points, $p = 50$, $p = 100$ and $p = 200$. Two functions α are considered, either $\alpha(t) = 10 \sin(2\pi t)$ or $\alpha(t) = 10 \sin^3(2\pi t^3)$. Finally, the error terms are chosen as follows: $\epsilon \sim \mathcal{N}(0, \sigma_\epsilon^2)$ with $\sigma_\epsilon = 0.2$ and $\delta(t_j) \sim \mathcal{N}(0, \sigma_\delta^2)$ for all $j = 1, \dots, p$ with either $\sigma_\delta = 0.1$, $\sigma_\delta = 0.2$ or $\sigma_\delta = 0.5$. Concerning the parameters of the spline functions, the order of differentiation in the penalization is fixed to the value $m = 2$. The most important parameter to choose is the smoothing one ρ (see [19]). We present in the next subsection a criterion allowing to make that choice, and we check the reliability of this criterion in the simulations.

5.2 Generalized Cross Validation criteria

In the Functional Least Squares estimation, ρ can be fixed by *Generalized Cross Validation* (*GCV*) as described in [27]. More precisely, we consider the *GCV* criterion defined by

$$GCV_{FLS,W}(\rho) = \frac{\frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{\left(1 - \frac{1}{n} \text{Tr}(\mathbf{H}_{FLS,W}(\rho))\right)^2}, \quad (26)$$

where $\mathbf{H}_{FLS,W}(\rho)$ is the “hat matrix” given by

$$\mathbf{H}_{FLS,W}(\rho) = \frac{1}{np} \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \mathbf{W}^\tau,$$

and $\hat{\mathbf{Y}} = \mathbf{H}_{FLS,W}(\rho) \mathbf{Y}$. Then, we select the optimal parameter ρ_{GCV} as the one that minimizes the *GCV* criterion (26).

Concerning the Functional Total Least Squares estimation, although *Cross Validation* has already been studied in [24], what we want to propose here is a generalization of the *GCV* criterion (26) above, in the following way. The prediction of Y_i for $i = 1, \dots, n$ is slightly different in the context of *TLS*. The estimation of the unknown \mathbf{X}_i , noted $\hat{\mathbf{X}}_i$, is given by

$$\widehat{\mathbf{X}}_i = \mathbf{W}_i + \frac{Y_i - \frac{1}{p}\widehat{\boldsymbol{\alpha}}^\tau \mathbf{W}_i}{1 + \frac{1}{p}\|\widehat{\boldsymbol{\alpha}}\|^2} \widehat{\boldsymbol{\alpha}}, \quad (27)$$

obtained as in [12] by differentiating equation (19) with respect to \mathbf{X}_i . Then, we take $\widehat{Y}_i = \langle \widehat{\boldsymbol{\alpha}}, \widehat{\mathbf{X}}_i \rangle_p$ as the prediction of Y_i . Then, the suggested *GCV* criterion is given by

$$GCV_{FTLS}(\rho) = \frac{\frac{1}{n} \sum_{i=1}^n (Y_i - \langle \widehat{\boldsymbol{\alpha}}_{FTLS}, \widehat{\mathbf{X}}_i \rangle_p)^2}{\left(1 - \frac{1}{n} \text{Tr}(\mathbf{H}_{FTLS}(\rho))\right)^2}, \quad (28)$$

where $\mathbf{H}_{FTLS}(\rho)$ is the “hat matrix” given by

$$\mathbf{H}_{FTLS}(\rho) = \frac{1}{np} \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \frac{\widehat{\sigma}_\delta^2}{p^2} \mathbf{I}_p \right)^{-1} \mathbf{W}^\tau$$

Then, we select the optimal parameters ρ_{GCV} as the one that minimize the *GCV* criterion (28). In practice, these *GCV* criteria have been computed for ρ taking its values among $10^{-2}, 10^{-3}, \dots, 10^{-8}$.

5.3 Results of the simulation

We use two error criteria to see the quality of the prediction. The first one is the relative mean square error of the estimator of $\boldsymbol{\alpha}$, given by

$$E_1 = \frac{\sum_{j=1}^p [\widehat{\boldsymbol{\alpha}}(t_j) - \boldsymbol{\alpha}(t_j)]^2}{\sum_{j=1}^p \boldsymbol{\alpha}(t_j)^2}, \quad (29)$$

and the second one is the mean square error of the prediction of \mathbf{Y} , given by

$$E_2 = \frac{1}{n} \sum_{i=1}^n \left(\widehat{Y}_i - Y_i \right)^2. \quad (30)$$

We have put in tables 1 and 2 the values of these errors computed on the $N = 100$ simulated test samples, for the different values of p and the different functions α . We have computed the *FLS* estimator of α using the unknown true curves X (in order to have a reference), the observed curves W and the smooth version \widetilde{W} of the observed curves W .

We can see that the *FTLS* estimator always improves the prediction compared to *FLS*, W , and the improvement is really interesting when p is small with a relatively important noise level σ_δ . We can also see that the estimators *FTLS* and *FLS*, \widetilde{W} are quite close. *FLS*, \widetilde{W} seems to be

better when the noise level σ_δ is small, and *FTLS* seems to be better when this noise level becomes high. Nevertheless, it is important to note that the *FTLS* estimator is faster to compute compared to the *FLS*, \widetilde{W} one. Indeed, choosing the parameter h by cross validation implies long computation times, above all when n is high (we have to compute n cross validation criteria).

Moreover, it has to be noticed that the prediction is also improved when the number of discretization points increases. We can also see that the error increases between table 1 and table 2, mainly because of the shape of the second function α , which is less smooth than the first one.

Table 3 gives the estimated values of σ_δ using the estimator defined by (22) and given in [13]. We can see that we get good estimations of σ_δ , and increasing with the number of discretization points. It also seems that the quality of the estimation is not much related to the value of σ_δ . Finally, we have plotted on figure 1 an example of the estimation of α in the case where $p = 100$ and $\sigma_\delta = 0.5$. In order not to have too many curves on a same graphic, we chose to plot only the estimators *FTLS*, *FLS*, X and *FLS*, W , the estimator *FLS*, \widetilde{W} being quite “close” from *FTLS*. This graphic tends to confirm the values given in tables 1 and 2. In the case where the function α to predict is smooth (case $\alpha(t) = 10 \sin(2\pi t)$), we can see on the graphic that there is a really slight difference between the three different estimators (*FTLS*, *FLS*, X and *FLS*, W).

Table 1 to be put here

Table 2 to be put here

Table 3 to be put here

Figure 1 to be put here

6 Proof of the results

6.1 Proof of theorem 1

First consider relation (14), and note that

$$\mathbb{E}(\hat{\alpha}_{FLS,X}) = \frac{1}{np^2} \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \mathbf{X}^\tau \mathbf{X} \alpha,$$

It follows that $\mathbb{E}(\hat{\alpha}_{FLS,X})$ is solution of the minimization problem

$$\min_{\alpha \in \mathbb{R}^p} \left\{ \frac{1}{n} \left\| \frac{1}{p} \mathbf{X} \alpha - \frac{1}{p} \mathbf{X} \mathbf{a} \right\|^2 + \frac{\rho}{p} \mathbf{a}^\tau \mathbf{A}_m \mathbf{a} \right\}.$$

This implies

$$\frac{1}{n} \left\| \frac{1}{p} \mathbf{X} \alpha - \frac{1}{p} \mathbf{X} \mathbb{E}(\hat{\alpha}_{FLS,X}) \right\|^2 + \frac{\rho}{p} \mathbb{E}(\hat{\alpha}_{FLS,X})^\tau \mathbf{A}_m \mathbb{E}(\hat{\alpha}_{FLS,X}) \leq \frac{\rho}{p} \alpha^\tau \mathbf{A}_m \alpha.$$

But definition of \mathbf{A}_m and as well (8) lead to

$$\frac{1}{p} \alpha^\tau \mathbf{A}_m \alpha = \frac{1}{p} \alpha^\tau \mathbf{P}_m \alpha + \int_I s_{\alpha}^{(m)}(t)^2 dt \leq \frac{1}{p} \alpha^\tau \mathbf{P}_m \alpha + \int_I \alpha^{(m)}(t)^2 dt,$$

and (14) is an immediate consequence.

Relation (15) follows from

$$\begin{aligned} & \frac{1}{p} \mathbb{E} \left([\hat{\alpha}_{FLS,X}^\tau - \mathbb{E}(\hat{\alpha}_{FLS,X}^\tau)] [\hat{\alpha}_{FLS,X} - \mathbb{E}(\hat{\alpha}_{FLS,X})] \right) \\ &= \frac{1}{p} \mathbb{E} \left(\frac{1}{n^2 p^2} \epsilon^\tau \mathbf{X} \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-2} \mathbf{X}^\tau \epsilon \right) \\ &= \frac{\sigma_\epsilon^2}{n} \text{Tr} \left[\left(\frac{1}{np} \mathbf{X}^\tau \mathbf{X} + \rho \mathbf{A}_m \right)^{-2} \frac{1}{np} \mathbf{X}^\tau \mathbf{X} \right] \\ &\leq \frac{\sigma_\epsilon^2}{n} \text{Tr} \left[\left(\frac{1}{np} \mathbf{X}^\tau \mathbf{X} + \rho \mathbf{A}_m \right)^{-1} \right] \leq \frac{\sigma_\epsilon^2}{n} \text{Tr} \left[(\rho \mathbf{A}_m)^{-1} \right] \leq \frac{\sigma_\epsilon^2}{n\rho} C_1. \end{aligned}$$

This completes the proof of Theorem 1.

6.2 Proof of proposition 1

The model writes matricially

$$\begin{cases} \mathbf{Y} = \frac{1}{p}\mathbf{X}\boldsymbol{\alpha} + \boldsymbol{\epsilon} \\ \mathbf{W} = \mathbf{X} + \boldsymbol{\delta}, \end{cases} \quad (31)$$

hence we obtain

$$\left(\left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right) - \left(\frac{\boldsymbol{\delta}}{p}, \boldsymbol{\epsilon} \right) \right) \begin{pmatrix} \boldsymbol{\alpha} \\ -1 \end{pmatrix} = 0, \quad (32)$$

which allows us now to write the minimisation problem (19) as follows

$$\min_{\left(\left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right) - \left(\frac{\boldsymbol{\delta}}{p}, \boldsymbol{\epsilon} \right) \right) \begin{pmatrix} \boldsymbol{\alpha} \\ -1 \end{pmatrix} = 0} \left\{ \frac{1}{n} \left\| \left(\frac{\boldsymbol{\delta}}{\sqrt{p}}, \boldsymbol{\epsilon} \right) \right\|_F^2 + \frac{\rho}{p} \mathbf{a}^\tau \mathbf{A}_m \mathbf{a} \right\},$$

where the notation $\|\cdot\|_F$ stands for the usual Frobenius norm, more precisely $\|\mathbf{A}\|_F^2 = \text{Tr}(\mathbf{A}^\tau \mathbf{A})$ for every matrix \mathbf{A} . Then, we are led to consider the minimization problem

$$\min_{\mathbf{C}\mathbf{x}=\mathbf{E}\mathbf{x}} \left\{ \frac{1}{n} \left\| \left(\frac{\boldsymbol{\delta}}{\sqrt{p}}, \boldsymbol{\epsilon} \right) \right\|_F^2 + \frac{\rho}{p} \mathbf{x}^\tau \mathbf{B}_m \mathbf{x} \right\}, \quad (33)$$

with $\mathbf{C} = \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right)$, $\mathbf{E} = \left(\frac{\boldsymbol{\delta}}{p}, \boldsymbol{\epsilon} \right)$, $\mathbf{x} = \begin{pmatrix} \boldsymbol{\alpha} \\ -1 \end{pmatrix}$ and $\mathbf{B}_m = \begin{pmatrix} \mathbf{A}_m & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix}$. If we denote $\boldsymbol{\gamma}$ the $(p+1) \times (p+1)$ matrix defined by

$$\boldsymbol{\gamma} = \begin{pmatrix} \text{diag}(1/\sqrt{p}, \dots, 1/\sqrt{p}) & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix},$$

we have

$$\begin{aligned} \frac{1}{n} \mathbf{x}^\tau \boldsymbol{\gamma}^\tau \left(\frac{\boldsymbol{\delta}}{\sqrt{p}}, \boldsymbol{\epsilon} \right)^\tau \left(\frac{\boldsymbol{\delta}}{\sqrt{p}}, \boldsymbol{\epsilon} \right) \boldsymbol{\gamma} \mathbf{x} &= \frac{1}{n} \mathbf{x}^\tau \mathbf{E}^\tau \mathbf{E} \mathbf{x} = \frac{1}{n} \mathbf{x}^\tau \mathbf{C}^\tau \mathbf{C} \mathbf{x} \\ &= \frac{1}{n} \mathbf{x}^\tau \boldsymbol{\gamma}^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right)^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right) \boldsymbol{\gamma} \mathbf{x}, \end{aligned}$$

and then we can see that the quantity

$$\begin{aligned} &\frac{1}{n} \mathbf{x}^\tau \boldsymbol{\gamma}^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right)^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right) \boldsymbol{\gamma} \mathbf{x} + \frac{\rho}{p} \mathbf{x}^\tau \mathbf{B}_m \mathbf{x} \\ &= \frac{1}{n} \mathbf{x}^\tau \boldsymbol{\gamma}^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right)^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right) \boldsymbol{\gamma} \mathbf{x} + \mathbf{x}^\tau \boldsymbol{\gamma}^\tau (\rho \mathbf{B}_m) \boldsymbol{\gamma} \mathbf{x} \end{aligned}$$

is minimized for \mathbf{x} eigenvector of the matrix

$$\begin{aligned}
& \frac{1}{n} \gamma^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right)^\tau \left(\frac{\mathbf{W}}{\sqrt{p}}, \mathbf{Y} \right) \gamma + \gamma^\tau (\rho \mathbf{B}_m) \gamma \\
&= \frac{1}{n} \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right)^\tau \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right) + \frac{\rho}{p} \mathbf{B}_m,
\end{aligned}$$

corresponding to the smallest non-zero eigenvalue, which is denoted σ_k^2 . Using the definition of this eigenvalue, we deduce that

$$\left(\frac{1}{n} \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right)^\tau \left(\frac{\mathbf{W}}{p}, \mathbf{Y} \right) + \frac{\rho}{p} \mathbf{B}_m \right) \hat{\mathbf{x}} = \sigma_k^2 \hat{\mathbf{x}}.$$

This gives, keeping the p first rows,

$$\hat{\boldsymbol{\alpha}} = \frac{1}{np} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \sigma_k^2 \mathbf{I}_p \right)^{-1} \mathbf{W}^\tau \mathbf{Y},$$

and the proof of the proposition 1 is now complete.

6.3 Proof of proposition 2

Using the fact that $W_i(t_j) = X_i(t_j) + \delta_i(t_j)$ for all $i = 1, \dots, n$ and $j = 1, \dots, p$, we can write

$$\frac{1}{n} \mathbf{W}^\tau \mathbf{W} = \frac{1}{n} \mathbf{X}^\tau \mathbf{X} + \left(\frac{1}{n} \sum_{i=1}^n M_{irs} \right)_{r,s=1,\dots,p}$$

where $M_{irs} = X_i(t_r) \delta_i(t_s) + \delta_i(t_r) X_i(t_s) + \delta_i(t_r) \delta_i(t_s)$. Let us now study this random variable M_{irs} . First, we have

$$\begin{aligned}
\mathbb{E}(M_{irs}) &= X_i(t_r) \mathbb{E}(\delta_i(t_s)) + \mathbb{E}(\delta_i(t_r)) X_i(t_s) + \mathbb{E}(\delta_i(t_r) \delta_i(t_s)) \\
&= \begin{cases} \sigma_\delta^2 & \text{if } r = s, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}$$

On the other hand, we have with hypotheses (H.2) and (H.3)

$$\begin{aligned}
& \sup_{r,s=1,\dots,p} \mathbb{E}(M_{irs}^2) \\
&= \sup_{r,s=1,\dots,p} \left\{ X_i(t_r)^2 \mathbb{E}(\delta_i(t_s)^2) + \mathbb{E}(\delta_i(t_r)^2) X_i(t_s)^2 \right. \\
&\quad \left. + \mathbb{E}(\delta_i(t_r)^2 \delta_i(t_s)^2) + 2X_i(t_r) X_i(t_s) \mathbb{E}(\delta_i(t_r) \delta_i(t_s)) \right\} \\
&= O(\sigma_\delta^2),
\end{aligned}$$

hence we deduce

$$\sup_{r,s=1,\dots,p} \left(\frac{1}{n} \sum_{i=1}^n M_{irs} \right) = \begin{cases} \sigma_\delta^2 + O_P \left(\frac{\sigma_\delta}{n^{1/2}} \right) & \text{if } r = s, \\ O_P \left(\frac{\sigma_\delta}{n^{1/2}} \right) & \text{otherwise.} \end{cases}$$

We can now conclude the proof of proposition 2. If we define \mathbf{R} such that

$$\left(\frac{1}{np^2} \sum_{i=1}^n M_{irs} \right)_{r,s=1,\dots,p} = \frac{\sigma_\delta^2}{p^2} \mathbf{I}_p + \mathbf{R},$$

then $\sup_{r,s=1,\dots,p} |R_{rs}| = O_P \left(\frac{\sigma_\delta}{n^{1/2}p^2} \right)$ and we get (see theorem 1.19 in [5])

$$\|\mathbf{R}\| = O_P \left(\frac{\sigma_\delta}{n^{1/2}p} \right).$$

6.4 Proof of theorem 2

Let us consider the random variable $Z_{ij} = \delta_i(t_j)Y_i$. Using the independence between Y_i and δ_i , we get $\mathbb{E}(Z_{ij}) = 0$ and

$$\sup_{j=1,\dots,p} \mathbb{E}(Z_{ij}^2) = \sup_{j=1,\dots,p} \mathbb{E}(\delta_i(t_j)^2) \mathbb{E}(Y_i^2) = O(\sigma_\delta^2),$$

from what we deduce that

$$\sup_{i=1,\dots,n} \sup_{j=1,\dots,p} |Z_{ij}| = O_P(\sigma_\delta).$$

Now we see that

$$\sup_{j=1,\dots,p} \left| \frac{1}{n} \sum_{i=1}^n Z_{ij} \right| = O_P \left(\frac{\sigma_\delta}{n^{1/2}} \right),$$

and then

$$\|\mathbf{V}\|^2 := \left\| \frac{1}{np} \mathbf{W}^\tau \mathbf{Y} - \frac{1}{np} \mathbf{X}^\tau \mathbf{Y} \right\|^2 = \sum_{j=1}^p \left(\frac{1}{np} \sum_{i=1}^n Z_{ij} \right)^2 = O_P \left(\frac{\sigma_\delta^2}{np} \right). \quad (34)$$

Noticing now the convergence result given in [13] of the estimator $\widehat{\sigma}_\delta^2$ of σ_δ^2 , defined by (22), we have

$$\widehat{\sigma}_\delta^2 = \sigma_\delta^2 + O_P \left(\frac{1}{n^{1/2}p} \right). \quad (35)$$

Then, using this and the result (21) of the proposition 2, we can write

$$\left(\frac{1}{np^2}\mathbf{W}^\tau\mathbf{W} + \frac{\rho}{p}\mathbf{A}_m - \frac{\hat{\sigma}_\delta^2}{p^2}\mathbf{I}_p\right)^{-1} = \left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m + \mathbf{R} - \frac{\hat{\sigma}_\delta^2 - \sigma_\delta^2}{p^2}\mathbf{I}_p\right)^{-1}.$$

Now, let \mathbf{T} be the $p \times p$ matrix defined by $\mathbf{T} = \mathbf{R} - \frac{\hat{\sigma}_\delta^2 - \sigma_\delta^2}{p^2}\mathbf{I}_p$. Using the result (35) and the fact that the norm of \mathbf{I}_p is 1, we deduce

$$\left\|\frac{\hat{\sigma}_\delta^2 - \sigma_\delta^2}{p^2}\mathbf{I}_p\right\| = O_P\left(\frac{1}{n^{1/2}p^3}\right).$$

If we recall the order of $\|\mathbf{R}\|$ given in proposition 2, we finally obtain

$$\left(\frac{1}{np^2}\mathbf{W}^\tau\mathbf{W} + \frac{\rho}{p}\mathbf{A}_m - \frac{\hat{\sigma}_\delta^2}{p^2}\mathbf{I}_p\right)^{-1} = \left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m + \mathbf{T}\right)^{-1}, \quad (36)$$

with

$$\|\mathbf{T}\| = O_P\left(\frac{\sigma_\delta}{n^{1/2}p}\right). \quad (37)$$

Now, determining the norm of the matrix $\left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m\right)^{-1}$, we get

$$\left\|\left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m\right)^{-1}\right\| = O_P\left(\frac{1}{\rho}\right). \quad (38)$$

Using the first inequality given in [8], we can write (with C strictly positive constant)

$$\begin{aligned} & \left\|\left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m + \mathbf{T}\right)^{-1} - \left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m\right)^{-1}\right\| \\ & \leq C \left\|\left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m\right)^{-1}\right\|^2 \|\mathbf{T}\|. \end{aligned}$$

Then, using relations (37) and (38), we obtain

$$\begin{aligned} & \left\|\left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m + \mathbf{T}\right)^{-1} - \left(\frac{1}{np^2}\mathbf{X}^\tau\mathbf{X} + \frac{\rho}{p}\mathbf{A}_m\right)^{-1}\right\| \\ & = O_P\left(\frac{\sigma_\delta}{n^{1/2}p\rho^2}\right). \end{aligned} \quad (39)$$

Finally, if we set

$$\mathbf{S} = \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m + \mathbf{T} \right)^{-1} - \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1},$$

then we have (with relations (36) and (39))

$$\left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m - \frac{\hat{\sigma}_\delta^2}{p^2} \mathbf{I}_p \right)^{-1} = \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} + \mathbf{S}, \quad (40)$$

$$\text{with } \|\mathbf{S}\| = O_P \left(\frac{\sigma_\delta}{n^{1/2} p \rho^2} \right).$$

Let us now write

$$\begin{aligned} & \|\hat{\boldsymbol{\alpha}}_{FTLS} - \hat{\boldsymbol{\alpha}}_{FLS,X}\| \\ &= \left\| \left[\left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} + \mathbf{S} \right] \left[\frac{1}{np} \mathbf{X}^\tau \mathbf{Y} + \mathbf{V} \right] \right. \\ & \quad \left. - \frac{1}{np} \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \mathbf{X}^\tau \mathbf{Y} \right\| \\ &\leq \left\| \left(\frac{1}{np^2} \mathbf{X}^\tau \mathbf{X} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \right\| \|\mathbf{V}\| + \|\mathbf{S}\| \left\| \frac{1}{np} \mathbf{X}^\tau \mathbf{Y} \right\| + \|\mathbf{S}\| \|\mathbf{V}\|. \quad (41) \end{aligned}$$

The last thing to compute here is $\left\| \frac{1}{np} \mathbf{X}^\tau \mathbf{Y} \right\|$. In the same way as we have done to obtain (34), we write

$$\left\| \frac{1}{np} \mathbf{X}^\tau \mathbf{Y} \right\|^2 = \sum_{j=1}^p \left(\frac{1}{np} \sum_{i=1}^n X_i(t_j) Y_i \right)^2.$$

Then, using the fact that $\sup_{j=1,\dots,p} \mathbb{E}(X_i(t_j) Y_i) = O(1)$ and the fact that $\sup_{j=1,\dots,p} \mathbb{E}(X_i(t_j)^2 Y_i^2) = O(1)$, we obtain

$$\sup_{i=1,\dots,n} \sup_{j=1,\dots,p} |X_i(t_j) Y_i| = O_P(1),$$

and then

$$\left\| \frac{1}{np} \mathbf{X}^\tau \mathbf{Y} \right\|^2 = O_P \left(\frac{1}{np} \right). \quad (42)$$

Now, coming back to the inequality (41), using the results (34) and (40) as well as relations (38) and (42), we get

$$\|\hat{\boldsymbol{\alpha}}_{FTLS} - \hat{\boldsymbol{\alpha}}_{FLS,X}\| = O_P \left(\frac{\sigma_\delta}{n^{1/2} p^{1/2} \rho} \right) + O_P \left(\frac{\sigma_\delta}{np^{3/2} \rho^2} \right).$$

Since $\lim_{n \rightarrow +\infty} \frac{1}{n^{1/2} p \rho} = 0$, we get $\|\hat{\alpha}_{FTLS} - \hat{\alpha}_{FLS,X}\| = O_P\left(\frac{\sigma_\delta}{n^{1/2} p^{1/2} \rho}\right)$ and the proof of theorem 2 is complete.

6.5 Proof of proposition 3

Let us expand the $MISE(\lambda)$,

$$MISE(\lambda) = \mathbb{E}(\hat{\alpha}(\lambda)^\tau \hat{\alpha}(\lambda)) - 2\alpha^\tau \mathbb{E}(\hat{\alpha}(\lambda)) + \alpha^\tau \alpha,$$

to deduce, using the matricial expression of $\hat{\alpha}(\lambda)$

$$\begin{aligned} \frac{\partial}{\partial \lambda} MISE(\lambda)|_{\lambda=0} &= 2\mathbb{E} \left[\frac{1}{n^2 p^2} \mathbf{Y}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-3} \mathbf{W}^\tau \mathbf{Y} \right. \\ &\quad \left. - \frac{1}{np} \alpha^\tau \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-2} \mathbf{W}^\tau \mathbf{Y} \right]. \end{aligned} \quad (43)$$

Now, using the fact that $\mathbf{Y} = \frac{1}{p} \mathbf{W} \alpha - \frac{1}{p} \delta \alpha + \epsilon$

$$\begin{aligned} &\frac{1}{np} \mathbf{Y}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} - \alpha^\tau \\ &= \frac{1}{np} \mathbf{Y}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} - \frac{1}{np^2} \alpha^\tau \mathbf{W}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \\ &= \frac{1}{np} \left[\frac{1}{p} \alpha^\tau \mathbf{W}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \right. \\ &\quad \left. - \frac{1}{p} \alpha^\tau \delta^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} + \epsilon^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} \right] \\ &\quad - \frac{1}{np} \left[\frac{1}{p} \alpha^\tau \mathbf{W}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \right]. \end{aligned}$$

Considering the quantity $\left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} - \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1}$, if we make an approximation at first order, we get

$$\begin{aligned} &\left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-1} - \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \\ &\approx - \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \left(\frac{\rho}{p} \mathbf{A}_m \right) \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1}, \end{aligned}$$

what gives us, coming back to relation (43)

$$\begin{aligned}
& \frac{\partial}{\partial \lambda} MISE(\lambda)|_{\lambda=0} \\
\approx & 2\mathbb{E} \left[-\frac{1}{n^2 p^3} \boldsymbol{\alpha}^\tau \mathbf{W}^\tau \mathbf{W} \left(\left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \frac{\rho}{p} \mathbf{A}_m \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \right) \right. \\
& \quad \left. \times \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-2} \mathbf{W}^\tau \mathbf{Y} \right] \\
& + 2\mathbb{E} \left[-\frac{1}{n^2 p^3} \boldsymbol{\alpha}^\tau \boldsymbol{\delta}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-3} \mathbf{W}^\tau \mathbf{Y} \right] \\
& + 2\mathbb{E} \left[\frac{1}{n^2 p^2} \boldsymbol{\epsilon}^\tau \mathbf{W} \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-3} \mathbf{W}^\tau \mathbf{Y} \right]. \tag{44}
\end{aligned}$$

Using the fact that δ and ϵ are both independent from W and Y , the last two terms in relation (44) are zero, and we obtain finally

$$\begin{aligned}
& \frac{\partial}{\partial \lambda} MISE(\lambda)|_{\lambda=0} \\
\approx & 2\mathbb{E} \left[-\frac{1}{n^2 p^4} \boldsymbol{\alpha}^\tau \mathbf{W}^\tau \mathbf{W} \left(\left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \frac{\rho}{p} \mathbf{A}_m \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} \right)^{-1} \right) \right. \\
& \quad \left. \times \left(\frac{1}{np^2} \mathbf{W}^\tau \mathbf{W} + \frac{\rho}{p} \mathbf{A}_m \right)^{-2} \mathbf{W}^\tau \mathbf{W} \boldsymbol{\alpha} \right].
\end{aligned}$$

This last quantity is negative, what achieves the proof of proposition 3.

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		E_1			E_2		
		$\sigma_\delta = 0.1$	$\sigma_\delta = 0.2$	$\sigma_\delta = 0.5$	$\sigma_\delta = 0.1$	$\sigma_\delta = 0.2$	$\sigma_\delta = 0.5$
FLS, X	$p = 50$	0.00015	0.00014	0.00013	0.0031	0.0032	0.0032
	$p = 100$	0.00009	0.00010	0.00009	0.0027	0.0026	0.0027
	$p = 200$	0.00005	0.00006	0.00004	0.0024	0.0026	0.0025
$FTLS$	$p = 50$	0.00018	0.00061	0.00232	0.0044	0.0067	0.0180
	$p = 100$	0.00013	0.00065	0.00219	0.0040	0.0063	0.0139
	$p = 200$	0.00009	0.00057	0.00204	0.0035	0.0056	0.0091
FLS, \widetilde{W}	$p = 50$	0.00017	0.00080	0.00245	0.0040	0.0065	0.0209
	$p = 100$	0.00011	0.00063	0.00226	0.0036	0.0062	0.0154
	$p = 200$	0.00006	0.00056	0.00210	0.0029	0.0056	0.0112
FLS, W	$p = 50$	0.00020	0.00098	0.00366	0.0050	0.0081	0.0305
	$p = 100$	0.00015	0.00079	0.00344	0.0045	0.0072	0.0245
	$p = 200$	0.00011	0.00063	0.00329	0.0039	0.0067	0.0124

Table 1: Error E_1 on α given by $\alpha(t) = 10 \sin(2\pi t)$ and error E_2 of prediction.

		E_1			E_2		
		$\sigma_\delta = 0.1$	$\sigma_\delta = 0.2$	$\sigma_\delta = 0.5$	$\sigma_\delta = 0.1$	$\sigma_\delta = 0.2$	$\sigma_\delta = 0.5$
FLS, X	$p = 50$	0.0508	0.0509	0.0510	0.0427	0.0426	0.0426
	$p = 100$	0.0504	0.0504	0.0503	0.0422	0.0423	0.0424
	$p = 200$	0.0503	0.0502	0.0502	0.0414	0.0414	0.0416
$FTLS$	$p = 50$	0.0513	0.0526	0.0630	0.0439	0.0491	0.0830
	$p = 100$	0.0509	0.0522	0.0618	0.0434	0.0476	0.0762
	$p = 200$	0.0506	0.0517	0.0607	0.0429	0.0460	0.0735
FLS, \widetilde{W}	$p = 50$	0.0510	0.0525	0.0645	0.0435	0.0490	0.0851
	$p = 100$	0.0507	0.0520	0.0627	0.0429	0.0475	0.0790
	$p = 200$	0.0504	0.0516	0.0614	0.0422	0.0458	0.0763
FLS, W	$p = 50$	0.0516	0.0530	0.0850	0.0447	0.0504	0.0960
	$p = 100$	0.0512	0.0527	0.0822	0.0442	0.0496	0.0889
	$p = 200$	0.0508	0.0521	0.0799	0.0438	0.0488	0.0834

Table 2: Error E_1 on α given by $\alpha(t) = 10 \sin^3(2\pi t^3)$ and error E_2 of prediction.

	$\sigma_\delta = 0.1$	$\sigma_\delta = 0.2$	$\sigma_\delta = 0.5$
$p = 50$	0.1141	0.2075	0.5034
$p = 100$	0.1011	0.2005	0.5005
$p = 200$	0.0999	0.1999	0.4999

Table 3: Estimated values of σ_δ according to the different values of σ_δ and the different values of p .

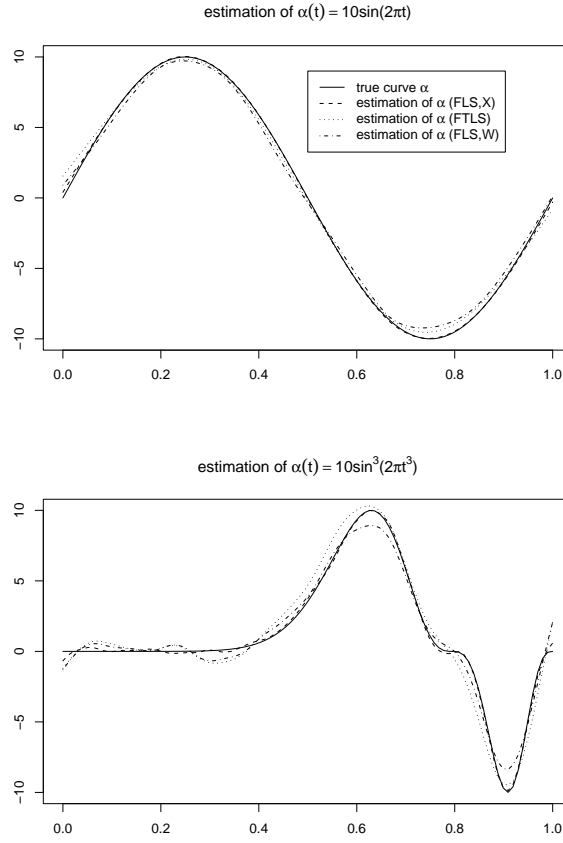


Figure 1: Estimation of α (solid line) with functional least squares using X (dashed line), functional least squares using W (dashed and dotted line) and functional total least squares (dotted line) in cases $\alpha(t) = 10 \sin(2\pi t)$ and $\alpha(t) = 10 \sin^3(2\pi t^3)$.