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Adaptive nonparametric estimation in the functional linear model with functional output

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Abstract

In this paper, we consider a functional linear regression model, where both the covariate and the response variable are functional random variables. We address the problem of optimal nonparametric estimation of the conditional expectation operator in this model. A collection of projection estimators over finite dimensional subspaces is first introduced. We provide a non-asymptotic bias-variance decomposition for the Mean Square Prediction error in the case where these subspaces are generated by the (empirical) PCA functional basis. The automatic trade-off is realized thanks to a model selection device which selects the best projection dimensions: the penalized contrast estimator satisfies an oracle-type inequality and is thus optimal in an adaptive point of view. These upper-bounds allow us to derive convergence rates over ellipsoidal smoothness spaces. The rates are shown to be optimal in the minimax sense: they match with a lower bound of the minimax risk, which is also proved. Finally, we conduct a numerical study, over simulated data and over two real-data sets.

1 Introduction

Functional data analysis (Ramsay and Silverman, 2005; Ferraty and Vieu, 2006; Ferraty and Romain, 2011) has attracted a growing interest from the past decades. In this context, regression models involving functional data as covariate are of particular interest. The case where the variable to predict is a real variable, called *functional linear model with scalar output* or simply *functional linear model* has been widely studied (see e.g. Cai et al. 2006; Cardot et al. 2007; Li and Hsing 2007; Hilgert et al. 2013; Cai and Yuan 2012) and is now well understood. In particular, the minimax rates for the estimation of the slope function in this model have been computed by Cardot and Johannes (2010) and adaptive estimators have been built (Comte and Johannes, 2010, 2012; Brunel and Roche, 2015; Brunel et al., 2016). On the contrary, the case of the *functional linear model with functional output*, where the variable to predict is also a functional variable has been less studied. This paper is dedicated to minimax adaptive estimation in this framework.

We assume here that we observe a sample $\{(X_i, Y_i), i = 1, \dots, n\}$, $n \in \mathbb{N} \setminus \{0\}$ of independent copies of a couple of functional data (X, Y) . For simplicity, we assume that both X and Y are random variables in the same functional space $\mathbb{H} = L^2([0, 1])$, the space of square integrable functions on the interval $[0, 1]$, equipped with its usual scalar product $\langle \cdot, \cdot \rangle$ defined by $\langle f, g \rangle = \int_0^1 f(t)g(t)dt$, $f, g \in \mathbb{H}$ and norm $\|\cdot\| = \sqrt{\langle \cdot, \cdot \rangle}$. The link between the functional variable of interest $Y \in \mathbb{H}$ and the functional covariate $X \in \mathbb{H}$ is linear: there exists an operator $S \in \mathcal{L}(\mathbb{H})$, the space of continuous linear operators on \mathbb{H} , such that

$$Y = SX + \varepsilon, \tag{1}$$

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where $\varepsilon \in \mathbb{H}$ stands for an (unobserved) noise. The functional variables X and ε are supposed to be both centered, and independent. The noise ε satisfied $\sigma_\varepsilon^2 = \mathbb{E}\|\varepsilon\|^2 < \infty$. The *slope operator* S is an integral operator and we denote by $\mathcal{S} \in L^2([0, 1]^2)$ its kernel:

$$\begin{aligned} S : \mathbb{H} &\longrightarrow \mathbb{H} \\ f &\longmapsto Sf : t \in [0, 1] \mapsto Sf(t) = \int_0^1 \mathcal{S}(s, t)f(s)ds. \end{aligned}$$

The aim is to estimate the unknown operator S (or its kernel \mathcal{S}) from the sample $(X_i, Y_i)_{i \in \{1, \dots, n\}}$.

It seems that the first article about estimation in this model is the one of [Cuevas et al. \(2002\)](#). In the fixed design case, they propose a histogram estimator and prove its consistency under strong assumption on the design matrix. A wavelets estimator has been considered by [Aguilera et al. \(2008\)](#) and a splines estimator by [Antoch et al. \(2010\)](#). The majority of the literature focus on estimators by projection onto the basis of principal components of the covariate X ([Chiou et al., 2004](#); [Yao et al., 2005](#)). The interest of functional Principal Components Analysis (PCA in the sequel) may be seen in the Karhunen-Loève decomposition of X that is to say the writing of X as a series (with convergence in \mathbb{H})

$$X = \sum_{j \geq 1} \sqrt{\lambda_j} \xi_j \varphi_j, \tag{2}$$

where $(\lambda_j)_{j \geq 1}$ is a non-increasing sequence of non-negative real numbers, $(\xi_j)_{j \geq 1}$ is a sequence of standardized random variables (the *principal components scores*) and $(\varphi_j)_{j \geq 1}$ is an orthonormal basis of \mathbb{H} (the *principal components basis*). It can be proved that, for a given dimension D , the space $\text{span}\{\varphi_1, \dots, \varphi_D\}$ is the best approximation space for X in the sense of the L^2 -loss i.e.

$$\text{span}\{\varphi_1, \dots, \varphi_D\} = \arg \min \{ \mathbb{E} [\|X - \text{proj}_S(X)\|^2], S \text{ lin. sub. of } \mathbb{H}, \dim(S) = D \}$$

where, for a linear subspace S of \mathbb{H} , $\text{proj}_S(X)$ is the orthogonal projection of X into S , see [Ferraty and Romain \(2011, Chapter 8\)](#) or [Hsing and Eubank \(2015, Theorem 7.2.8\)](#). We also refer to [Dauxois et al. \(1982\)](#); [Mas and Ruymgaart \(2015\)](#) for other reviews on PCA for functional data. A procedure to estimate the φ_j 's is described in [Section 2.2.2](#).

To our knowledge, few articles investigate the theoretical properties of slope operator or kernel estimators in [Model \(1\)](#). [Crambes and Mas \(2013\)](#) study an estimator of the slope operator S by projection onto the principal components basis. They provide a bias-variance decomposition of the mean squared prediction risk and compute optimal rates of convergence: such type of results can be stated only under some smoothness assumptions on the target operator S (as usual in nonparametric estimation) but also under assumptions of the process X , through the rate of decay of the eigenvalues (the λ_j 's in [\(2\)](#)) of the associated covariance operator. [Crambes and Mas \(2013\)](#) also derive weak convergence properties of their estimator. In their procedure, the smoothness indices of the target operator and of the covariate X (the decreasing rate of the covariance operator eigenvalues for example) are required to choose the projection dimension that permits to achieve the optimal rate. Thus, the method is not adaptive. More recently, [Imaizumi and Kato \(2018\)](#) study two estimation procedures called *simple* and *double* truncature. The simple truncature estimator corresponds to the one of [Crambes and Mas \(2013\)](#). They obtain lower and asymptotic upper-bounds on the estimation risk of the slope kernel \mathcal{S} . As in [Crambes and Mas \(2013\)](#), the procedure is not adaptive, and the results are valid only when the decay rate of the eigenvalues of the covariance operator is a polynomial one.

In the present work, we propose a procedure which leads to an optimal estimate for the slope operator in [Model \(1\)](#), both from the minimax and the adaptive estimation point of view, for the mean squared prediction error. We first introduce a collection of projection estimators, by minimizing a least-squares contrast function over subspaces of \mathbb{H} spanned by the first elements of the PCA basis, corresponding to the *double truncature* procedure of [Imaizumi and Kato \(2018\)](#). We focus on the mean squared prediction error and compute a non-asymptotic upper-bound in [Theorem 3](#). This bound exhibits a bias-variance decomposition allowing us to derive rates of convergence, under some regularity assumption on the operator $ST^{1/2}$ (see [Corollary 1](#)). We then show that these bounds match with lower bounds that we also proved in [Theorem 2](#) (see also [Corollary 2](#)). One of the other main original contributions of this paper is to propose an entirely data-driven procedure to automatically select the best projection dimensions. The method relies on classical model selection tools ([Massart, 2007](#)), and takes advantage

of the definition of the estimates as minimized-contrast estimators. A penalized version of the contrast function permits to derive data driven estimate, which satisfies an oracle-type inequality, and achieves the optimal minimax convergence rates. Our selection rule does not depend on smoothness parameters of X and S . The procedure is then adaptive and minimax optimal.

The paper is organized as follows. Our least-squares estimators are constructed in Section 2. Upper and lower-bounds for the risk we choose are established in Section 3, after the description of the main hypotheses. Section 4 is devoted to adaptive estimation: the penalization strategy is described, and the oracle inequality as well as adaptive convergence rates are stated. Numerical results illustrate the theoretical properties in Section 5. We first calibrate our estimator and study its performances on simulated data in Section 5.1. Then we apply our procedure on two real-data sets problems in Section 5.2: the prediction of the appliances electricity consumption of a day given the ones of the day before (Candanedo et al., 2017), and the prediction of the evolution of the electricity prices from the wind power in-feed (Liebl, 2013). Finally, the proofs are gathered in Section 6.

2 Estimation method

2.1 Notations

We introduce here some notations which will be used all along this document. We denote by $\mathcal{L}_2(\mathbb{H})$ the subspace of Hilbert-Schmidt operators on \mathbb{H} equipped with its usual Hilbert-Schmidt norm defined for any operator $T \in \mathcal{L}_2(\mathbb{H})$ as follows

$$\|T\|_{\text{HS}} = \left(\sum_{j=1}^{\infty} \|T\phi_j\|^2 \right)^{1/2},$$

where $(\phi_j)_{j \geq 1}$ is a Hilbertian basis of \mathbb{H} . Note that the Hilbert-Schmidt norm is independent of the Hilbertian basis choice. It is also worth mentioning that an integral operator is Hilbert-Schmidt if and only if the associated kernel is square integrable. This means that by assumptions, our target operator S is Hilbert-Schmidt. We also need to define two operators that play a key role in the estimation procedure, namely the covariance and cross-covariance operators. To do so, we first define the tensor product between two elements a and b of \mathbb{H} as

$$\begin{aligned} b \otimes a : \mathbb{H} &\longrightarrow \mathbb{H} \\ f &\longmapsto \langle a, f \rangle b. \end{aligned}$$

The covariance operator of X , denoted Γ is the operator defined by

$$\begin{aligned} \Gamma : \mathbb{H} &\longrightarrow \mathbb{H} \\ f &\longmapsto \mathbb{E}[X \otimes X(f)] = \mathbb{E}[\langle X, f \rangle X]. \end{aligned}$$

Note that the covariance operator is a natural extension of the covariance matrix, in the infinite-dimensional framework. The $(\lambda_j, \varphi_j)_j$ involved in (2) are the eigenelements of Γ . We also introduce the cross-covariance operator Δ of (X, Y) given by

$$\begin{aligned} \Delta : \mathbb{H} &\longrightarrow \mathbb{H} \\ f &\longmapsto \mathbb{E}[Y \otimes X(f)] = \mathbb{E}[\langle X, f \rangle Y]. \end{aligned}$$

Empirical counterparts of Γ and Δ , respectively denoted by Γ_n and Δ_n will be useful in the definition of our estimators. These operators are naturally defined on \mathbb{H} by

$$\Gamma_n = \frac{1}{n} \sum_{i=1}^n X_i \otimes X_i \quad \text{and} \quad \Delta_n = \frac{1}{n} \sum_{i=1}^n Y_i \otimes X_i.$$

In order to study the estimator behaviors, we use an optimality risk called the Mean Square Prediction Error (MSPE). This criterion is also used in Crambes and Mas (2013); Cardot and Johannes (2010); Crambes et al. (2009) or Brunel et al. (2016). The MSPE of a given estimator \hat{S} of S is defined as

$$\text{MSPE}(\hat{S}_n) = \mathbb{E} \|\hat{S}_n(X_{n+1}) - S(X_{n+1})\|^2,$$

where X_{n+1} is a new observation of X , independent of $(X_i, \varepsilon_i), i = 1, \dots, n$. This risk can also be written

$$\text{MSPE}(\widehat{S}_n) = \mathbb{E} \left[\|\widehat{Y}_{n+1} - \mathbb{E}[Y_{n+1}|X_{n+1}]\|^2 | (X_i, Y_i)_{i=1, \dots, n} \right], \quad (3)$$

where $Y_{n+1} = SX_{n+1} + \varepsilon_{n+1}$, $\widehat{Y}_{n+1} = \widehat{S}_n X_{n+1}$, and $\mathbb{E}[\cdot|Z]$ is the conditional expectation given a variable Z . It is also linked with the Hilbert-Schmidt norm as follows,

$$\mathbb{E}\|\widehat{S}_n(X_{n+1}) - S(X_{n+1})\|^2 = \mathbb{E}\|(\widehat{S}_n - S)\Gamma^{1/2}\|_{\text{HS}}^2, \quad (4)$$

see Lemma 5 in the proof (Section 6.3).

For two sequences $(a_j)_{j \geq 1}$ and $(b_j)_{j \geq 1}$ of real numbers, we write $a_j \asymp b_j$ if there exists $c \geq 1$ such that $c^{-1}a_j \leq b_j \leq ca_j$.

2.2 Least-squares estimation

2.2.1 Minimum contrast estimation

The main goal of statistical estimation is to build an estimate that leads to a small risk. Following the model selection device introduced by Birgé et al. (1998), we minimize an empirical counterpart of the risk, called the contrast function, over finite dimensional subspaces of $\mathcal{L}_2(\mathbb{H})$, to build projection-type estimators. Let $(\phi_j)_{j \geq 1}$ be an orthonormal basis of $\mathbb{H} = L^2([0, 1])$. We introduce a collection of finite linear subspaces of $\mathcal{L}_2(\mathbb{H})$, called the models and denoted V_{m_1, m_2} for given m_1, m_2 in $\mathbb{N} \setminus \{0\}$. These models are defined as

$$V_{m_1, m_2} = \text{Span}\{\phi_k \otimes \phi_j, 1 \leq j \leq m_1, 1 \leq k \leq m_2\}.$$

Note that V_{m_1, m_2} only contains integral operators. Subsequently, for any $T \in \mathcal{L}_2(\mathbb{H})$, let

$$\gamma_n(T) = \frac{1}{n} \sum_{i=1}^n \|Y_i - T(X_i)\|^2.$$

The operator $\gamma_n : \mathcal{L}_2(\mathbb{H}) \rightarrow \mathbb{R}$ is defined in the spirit of other regression contrast introduced for example by Baraud (2002) and Brunel et al. (2016) and stands for an empirical version of the risk (3). Thus, we set

$$\widehat{S}_{m_1, m_2} \in \arg \min_{T \in V_{m_1, m_2}} \gamma_n(T). \quad (5)$$

To compute \widehat{S}_{m_1, m_2} , we introduce the matrices A and Y_ϕ given by

$$A = (\langle \Gamma_n \phi_j, \phi_k \rangle)_{j, k \in \{1, \dots, m_1\}} \quad \text{and} \quad Y_\phi = (\langle \Delta_n \phi_j, \phi_k \rangle)_{j \in \{1, \dots, m_1\}, k \in \{1, \dots, m_2\}}.$$

The following result, which proof can be found in Section 6.1.1, gives a condition for the existence of \widehat{S}_{m_1, m_2} .

Proposition 1. *If the matrix A is invertible, then \widehat{S}_{m_1, m_2} in (5) is uniquely defined, and*

$$\widehat{S}_{m_1, m_2} = \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} \widehat{b}_{j, k} \phi_k \otimes \phi_j,$$

with $\widehat{b} = (\widehat{b}_{j, k})_{j \in \{1, \dots, m_1\}, k \in \{1, \dots, m_2\}}$ defined by $\widehat{b} = A^{-1}Y_\phi$.

Remark 1. *Since S is an integral operator with kernel \mathcal{S} , we could also have defined a contrast function over the space of the kernel functions: for any $\mathcal{T} \in L^2([0, 1]^2)$, let*

$$\gamma'_n(\mathcal{T}) = n^{-1} \sum_{i=1}^n \|Y_i - \int_{[0, 1]} \mathcal{T}(s, \cdot) X(s) ds\|^2.$$

If we denote by $V'_{m_1, m_2} = \text{Span}\{(t, s) \mapsto \phi_j(s)\phi_k(t), 1 \leq j \leq m_1, 1 \leq k \leq m_2\}$, we can set $\widehat{S}_{m_1, m_2} \in \arg \min_{\mathcal{T} \in V'_{m_1, m_2}} \gamma'_n(\mathcal{T})$. The estimator \widehat{S}_{m_1, m_2} is also uniquely defined under the assumptions of Proposition 1, and for any $f \in \mathbb{H}$,

$$\widehat{S}_{m_1, m_2} f = \int_0^1 \widehat{\mathcal{S}}_{m_1, m_2}(s, \cdot) f(s) ds. \quad (6)$$

Remark 2. Defined with (5), \widehat{S}_{m_1, m_2} estimates the orthogonal projection $\Pi_{m_1, m_2}^{op} S$ of the operator S onto the operator space V_{m_1, m_2} . This projection operator can be written, for any $T \in \mathcal{L}_2(\mathbb{H})$,

$$\Pi_{m_1, m_2}^{op} T = \Pi_{m_1} T \Pi_{m_2}, \quad (7)$$

where, for any $m \in \mathbb{N} \setminus \{0\}$, Π_m is the projection operator on the subspace $\text{Span}\{\phi_k, k \in \{1, \dots, m\}\}$. The proof of (7) can be found in Section 6.1.2.

2.2.2 Specific choice of the projection spaces : principal component basis

In the rest of this article, we focus on the basis of principal components. Recall that, by definition, the empirical covariance operator Γ_n is self-adjoint. Moreover, since it is a finite-rank operator, it is also a compact operator. Then Γ_n is diagonalisable in a Hilbertian basis, denoted by $(\widehat{\varphi}_j)_{j \geq 1}$. We also denote by $(\widehat{\lambda}_j)_{j \geq 1}$ its eigenelements, which are sorted in a decreasing order. The $(\widehat{\varphi}_j)_{j \geq 1}$ is called the empirical PCA basis of X . Notice that the operator Γ_n is not invertible, since it has finite rank at most equal to n . This means that the eigenvalues $(\widehat{\lambda}_j)_{j \geq 1}$ are zero from a given rank. Let us introduce its pseudo-inverse, Γ_{n, m_1}^\dagger , defined for an index $m_1 \in \mathbb{N} \setminus \{0\}$ by

$$\Gamma_{n, m_1}^\dagger = \sum_{j=1}^{m_1} \frac{1}{\widehat{\lambda}_j} \widehat{\varphi}_j \otimes \widehat{\varphi}_j,$$

for $m_1 \leq m_{\max}$, with $m_{\max} = \max_{m \geq 1} \{\widehat{\lambda}_m > 0\}$ is the rank from which the eigenvalues are equal to zero, and $\Gamma_{n, m_1}^\dagger = \Gamma_{n, m_{\max}}^\dagger$ for $m_1 > m_{\max}$.

We obtain the following expressions for the least-squares estimators of the linear operator S and its kernel \mathcal{S} . The proof can be found in Section 6.1.3.

Proposition 2. *On the PCA basis, the least-squares estimator for the kernel \mathcal{S} exists, and is uniquely defined by*

$$\widehat{S}_{m_1, m_2}(s, t) = \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} \frac{1}{\widehat{\lambda}_j} \langle \Delta_n \widehat{\varphi}_j, \widehat{\varphi}_k \rangle \widehat{\varphi}_j(s) \widehat{\varphi}_k(t), \quad (s, t) \in [0, 1]^2. \quad (8)$$

Moreover, the expression of the resulting estimator for the linear operator S is

$$\widehat{S}_{m_1, m_2} = \Delta_n \Gamma_{n, m_1}^\dagger + \sum_{\substack{1 \leq j \leq m_1 \\ 1 \leq k \leq m_2 \\ j \neq k}} \frac{1}{\widehat{\lambda}_j} \langle \Delta_n \widehat{\varphi}_j, \widehat{\varphi}_k \rangle \widehat{\varphi}_j \otimes \widehat{\varphi}_k. \quad (9)$$

Remark that our estimator can also be written $\widehat{S}_{m_1, m_2} = \widehat{\Pi}_{m_2} \Delta_n \Gamma_{n, m_1}^\dagger$, where $\widehat{\Pi}_{m_2}$ is the projection operator onto the finite dimensional subspace $\text{Span}\{\widehat{\varphi}_k, k = 1, \dots, m_2\}$. Thus, \widehat{S}_{m_1, m_2} can be compared to the estimator of Crambes and Mas (2013) which writes $\widehat{S}_{m_1}^{CM} = \Delta_n \Gamma_{n, m_1}^\dagger$. Our choice is based on the fact that the initial regression problem comes down to estimate the kernel $\mathcal{S} \in L^2([0, 1]^2)$ of the operator S , which brings out two projection dimensions. Our estimate is thus the same as the estimator with “double truncation” of Imaizumi and Kato (2018) (see their equation (7) p.19), even if they do not introduce it as a minimum of contrast estimator. The definition of \widehat{S}_{m_1, m_2} as an operator that minimizes a contrast allows us to derive non-asymptotic upper-bounds for the prediction error, and to propose a data-driven way to select the best projection dimensions.

3 Upper and lower bounds of the estimation risk

In this section, we provide sharp upper bounds for the estimation risk of the estimator \widehat{S}_{m_1, m_2} , for any but fixed $(m_1, m_2) \in (\mathbb{N} \setminus \{0\})^2$, after stating the main hypotheses. We also establish a lower bound for the prediction risk, to ensure that the collection of estimates is reasonable.

3.1 Assumptions

Classically, we need to make some assumptions for optimal theoretical results. We distinguish different types of assumptions: regularity assumptions on $S\Gamma^{1/2}$, regularity assumptions on X , moment assumptions on X and moment assumptions on the noise ε .

Assumption on $S\Gamma^{1/2}$: We consider by analogy with Brunel et al. (2016), the regularity space of type ellipsoid, defined for all positive α, β, R by

$$\mathcal{W}_{\alpha, \beta}^R = \left\{ T \in \mathcal{L}_2(\mathbb{H}), \sum_{j=1}^{+\infty} \sum_{r=1}^{+\infty} \eta_\alpha(j) \psi_\beta(r) \langle T(\varphi_j), \varphi_r \rangle^2 \leq R^2 \right\},$$

where $\alpha, \beta > 0$ and for all $\gamma > 0$, the functions η_γ is defined such that

$$\eta_\gamma(j) \asymp j^\gamma \text{ or } \eta_\gamma(j) \asymp \exp(j^\gamma),$$

and the same for ψ_γ . We speak about the ‘‘polynomial case’’ or the ‘‘exponential case’’ in the sequel. These regularity spaces are generalization of the ellipsoid sets in the finite dimensional framework. Moreover, the regularity parameters α and β are respectively the convergence rates towards 0 of the operator components in both directions.

\mathcal{A}_1 : We assume that $S\Gamma^{1/2}$ belongs to $\mathcal{W}_{\alpha, \beta}^R$ for some positive regularity parameters α, β, R .

Assumption **\mathcal{A}_1** is a smoothness assumption on the operator S we want to recover. In nonparametric estimation, it is classical, and permits to control the bias term of the risk and to derive convergence rates (see *e.g.* Tsybakov (2008)). The kind of smoothness ball (ellipsoid space) we choose is also classical for projection type estimation (again, see Tsybakov (2008), but also Barron et al. (1999), or Brunel et al. (2016)).

The specificity of our assumption is that it is a joint regularity assumption both on S and on the covariate X . This technical choice is related to the choice of the mean squared prediction error we consider in this work: this risk is linked to the Hilbert-Schmidt norm of $S\Gamma^{1/2}$, see (4), it is thus natural that the smoothness assumption refers to this operator. This was also the case in the paper of Crambes and Mas (2013) and was pointed out by Hilgert et al. (2013). In a similar but different way same discussions appear in Comte and Johannes (2012): the link between the smoothness of S and X appears in a ‘‘compatibility’’ assumption on the norms, see their section 3.1. If we replace the prediction risk with a quadratic risk, the most appropriate choice would be to impose a regularity assumption only on S , as done in Imaizumi and Kato (2018).

Assumptions on X : Requiring a regularity on X is tantamount to making assumptions on Γ and its eigenvalues $(\lambda_j)_{j \geq 1}$. In particular, we consider that the eigenvalues are all distincts. In addition, we assume the following,

\mathcal{A}_2 : For all j in $\mathbb{N} \setminus \{0\}$, we have $\lambda_j \psi_\beta(j) \geq 1$.

The previous assumption ensures a separability condition on the eigenvalues of Γ . Indeed, considering that the model estimation is based on the estimation of the eigenfunctions of Γ_n , a separability condition on the eigenvalues of Γ , ensuring that they are not too close to each others is needed. Separation conditions on the eigenvalues of the covariance operator are usual in functional PCA regression. A usual alternative is to consider assumptions on the gap between two consecutive eigenvalues, as in Imaizumi and Kato (2018) or Hall and Horowitz (2007).

\mathcal{A}_3 : There exists a convex positive function $x \mapsto \lambda(x)$ such that, for all j in $\mathbb{N} \setminus \{0\}$: $\lambda_j = \lambda(j)$.

\mathcal{A}_4 : There exists a constant $\gamma > 0$ for which the sequence $(j \lambda_j \max\{\ln^{1+\gamma}(j), 1\})_{j \geq 1}$ decreases.

Assumptions **\mathcal{A}_3** and **\mathcal{A}_4** permits to obtain some decreasing rate of convergence of the eigenvalues of Γ and are classical in obtaining the optimal convergence rate of estimation. Similar assumptions have also been made in Crambes and Mas (2013) and Brunel et al. (2016).

Moment assumptions on X :

\mathcal{A}_5 : There exists a constant $b > 0$ such that, for all l in $\mathbb{N} \setminus \{0\}$,

$$\sup_{j \geq 1} \mathbb{E} \left[\frac{\langle X, \varphi_j \rangle^{2l}}{\lambda_j^l} \right] \leq l! b^{l-1}.$$

Like Assumption \mathcal{A}_3 , one can also find Assumption \mathcal{A}_5 in [Crambes and Mas \(2013\)](#) and [Brunel et al. \(2016\)](#). The control of the moment of the random variables $\langle X, \varphi_j \rangle$, $j \geq 1$ is required to apply Bernstein's exponential inequality.

\mathcal{A}_6 : For all $j \neq k$, $\langle X, \varphi_j \rangle$ and $\langle X, \varphi_k \rangle$ are independent.

Both assumptions \mathcal{A}_5 and \mathcal{A}_6 are satisfied when X is a Gaussian process (see [Ash and Gardner 1975](#), Section 1.4). For general (non Gaussian) processes, we know that $\langle X, \varphi_j \rangle$ and $\langle X, \varphi_k \rangle$ are, at least, uncorrelated since $\mathbb{E}[\langle X, \varphi_j \rangle \langle X, \varphi_k \rangle] = \langle \Gamma \varphi_j, \varphi_k \rangle = \lambda_j \mathbf{1}_{\{j=k\}}$.

Moment assumption on ε :

\mathcal{A}_7 : There exists $p > 6$ such that $\tau_p = \mathbb{E}\|\varepsilon\|^p < +\infty$.

The moment assumption \mathcal{A}_7 is classically needed to obtain adaptive estimators of the model S . Indeed, when no assumption is imposed on the fluctuation of noise, it is not possible to construct optimal estimator without knowing the regularity of the model. We can deduce easily, e.g. from [Chagny and Roche \(2014, Lemma 8\)](#), that it is verified if $\mathbb{E}[\|\varepsilon\|^2] < +\infty$ and $\mathbb{E}[\langle \varepsilon, f \rangle^p] < +\infty$, for all $f \in \mathbb{H}$. As particular cases, \mathcal{A}_7 is verified as soon as the noise is Gaussian, or bounded.

3.2 Upper bound of the Mean Square Prediction Error (MSPE)

Theorem 1 below gives a first sharp upper bound of the Mean Squared Prediction Error of the estimator \widehat{S}_{m_1, m_2} with respect to the projection dimensions m_1 and m_2 . This permits to have (up to a positive constant) an order of magnitude of the prediction error for each theoretical choice of m_1 and m_2 . The proof of the results of the section can be found in Section 6.3.

Theorem 1. *Under Assumptions \mathcal{A}_1 to \mathcal{A}_6 , the Mean Squared Prediction Error of the estimator \widehat{S}_{m_1, m_2} is upper bounded by*

$$\text{MSPE}(\widehat{S}_{m_1, m_2}) \leq \sigma_\varepsilon^2 \frac{m_1}{n} + 3 \sum_{j=m_1+1}^{+\infty} \|ST^{1/2}(\varphi_j)\|^2 + 3 \sum_{j=1}^{m_1} \|(I - \Pi_{m_2})ST^{1/2}(\varphi_j)\|^2 + A_{n, m_1} + B_{n, m_1} + D_{n, m_2} + E_n, \quad (10)$$

where, for a constant C which does not depend on n , m_1 , m_2 ,

$$A_{n, m_1} = \sigma_\varepsilon^2 \frac{C m_1^2 \ln^2(m_1)}{n^2}, \quad B_{n, m_1} = \frac{C m_1^2 \lambda_{m_1} \|S\|_{\text{HS}}}{n}, \quad E_n = \frac{C}{n^2} \|ST^{1/2}\|_{\text{HS}}^2$$

$$D_{n, m_2} = \frac{C m_2 \lambda_{m_2}}{n} + \frac{C m_2^2 \ln(m_2)}{n \psi_\beta(m_2)} + \frac{C m_2^3}{n \psi_\beta(\lfloor m_2/2 \rfloor)} + \frac{C \ln^4(n)}{n^2} \left(\sum_{k=1}^{m_2} \frac{k^2 \ln^2(k)}{\sqrt{\psi_\beta(k)}} \right)^2.$$

In Theorem 1 appears a bias-variance trade-off. The first term in the right side of Equation (10) is a variance term, which increases with m_1 . The two following terms are bias terms: one is decreasing with m_1 , the other one with m_2 . Both are related to the smoothness of $ST^{1/2}$. Notice right now that it is not the smoothness of the target function S that influences the result, but the one of $ST^{1/2}$. This is consistent with the choice of the risk, since the prediction error we study can also be written

$$\text{MSPE}(\widehat{S}_{m_1, m_2}) = \mathbb{E}\|(\widehat{S}_{m_1, m_2} - S)\Gamma^{1/2}\|_{\text{HS}}^2,$$

see Lemma 5 below. The same phenomenon occurs for [Crambes and Mas \(2013\)](#). Compared to their result for the estimator $\widehat{S}_{m_1}^{CM}$ (see Theorem 2 p.2633 in [Crambes and Mas 2013](#)), the first two terms of the bias-variance decomposition (10) are the same, but we have an additional bias term (third term in the right-hand-side of (10)), which depends on the index m_2 . We prove in Corollary 1 below that the other terms are negligible.

Corollary 1. *Assume that we are in the case where the function ψ_β is polynomial with $\beta > 6$ or exponential. Assume also that there exists $\nu > 0$ such that $\lambda_j \leq j^{-1-\nu}$, for any $j \geq 1$. Under the assumptions of Theorem 1, we have the following bound of the non-asymptotic maximal prediction risk of \widehat{S}_{m_1, m_2} .*

$$\inf_{\substack{m_1, m_2 \in \mathbb{N} \setminus \{0\} \\ m_1 \leq n / \ln^2(n)}} \sup_{ST^{1/2} \in \mathcal{W}_{\alpha, \beta}^R} \text{MSPE}(\widehat{S}_{m_1, m_2}) \leq \inf_{\substack{m_1 \in \mathbb{N} \setminus \{0\} \\ m_1 \leq n / \ln^2(n)}} \left\{ \sigma_\varepsilon^2 \frac{m_1}{n} + \frac{3}{\eta_\alpha(m_1)} \right\} + \frac{c}{n}, \quad (11)$$

where c is a positive constant.

Some comments are needed at this point. The dimension parameter m_2 does not appear in the upper-bound. A similar phenomenon has been observed by [Imaizumi and Kato \(2018\)](#). It is mainly due to the fact that the variance is completely independent of it. Hence, since the bias decreases to 0 when $m_2 \rightarrow +\infty$, it is sufficient to choose m_2 sufficiently large so that the bias is negligible (remind that the estimator is well defined even in the case $m_2 = +\infty$).

Notice also that the additional assumption $\lambda_j \leq j^{-1-\nu}$ is very mild and useful only for technical purpose (we recall that, since the operator Γ is trace-class, $\sum_{j \geq 1} \lambda_j < +\infty$). It is satisfied if the eigenvalues decrease at a polynomial or exponential rate. It can also be relaxed to allow us to choose $\lambda_j = (j \ln^\mu(j))^{-1}$ for some $\mu \geq 1$.

Corollary 1 gives the sharpest possible upper-bound of the prediction risk for the estimator we define by projection onto the basis of principal components. In the next section, we show that the upper-bound of Corollary 1 is optimal over the ellipsoidal regularity spaces we consider here.

3.3 Lower bound of the minimax Mean Square Prediction risk

In this section, we demonstrate that the upper-bound of the Mean Square Prediction risk obtained in Corollary 1 is optimal in the minimax sense in a non-asymptotic framework. This result is stated in Theorem 2 below. The demonstration of this result is based on a reduction scheme to a finite number of hypotheses, as explained in [Tsybakov \(2008\)](#). We apply the Kullback-Leibler version of Assouad's Lemma, and the Cameron-Martin theorem ([Lifshits, 2012](#)). It permits to control the likelihood expectation between different possible data distributions in the finite model collection.

Theorem 2. *Let $\alpha > 0$, $\beta > 0$ and $R > 0$, we have the following lower bound, for a constant $C > 0$,*

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha,\beta}^R} \text{MSPE}(\widehat{S}_n) \geq C \inf_{m_1 \in \mathbb{N} \setminus \{0\}} \left\{ \sigma_\varepsilon^2 \frac{m_1}{n} + \frac{3}{\eta_\alpha(m_1)} \right\},$$

where the infimum is taken over all estimators \widehat{S}_n calculated from a sample $\{(X_i, Y_i), i = 1, \dots, n\}$ following model (1), under the assumption that the noise ε is a Gaussian process.

This lower bound permits to derive the minimax explicit convergence rates in the polynomial and exponential cases.

Corollary 2. *Under the assumptions of Theorem 2, we compute the two following convergence decay for the minimax estimation risk, up to a constant $C > 0$.*

1. If $\eta_\alpha(j) \asymp j^\alpha$ (polynomial case) then,

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha,\beta}^R} \text{MSPE}(\widehat{S}_n) \geq C n^{-\frac{\alpha}{\alpha+1}}.$$

2. If $\eta_\alpha(j) \asymp \exp(j^\alpha)$ (exponential case) then,

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha,\beta}^R} \text{MSPE}(\widehat{S}_n) \geq C \frac{(\ln(n))^{1/\alpha}}{n}.$$

From Corollaries 1 and 2, we deduce that the projection estimators onto the PCA bases achieve the minimax rate for a suitable choice of the dimension m_1 and $m_2 = +\infty$. For example, it can be deduced in the polynomial case, that the optimal sharp upper-bound in Corollary 1 is obtained for $m_1 = C n^{1/(1+\alpha)}$ and $m_2 \rightarrow \infty$, where C is a universal positive constant. This leads to an upper-bound of order $n^{-\alpha/(\alpha+1)}$, which effectively matches with the lower bound of Corollary 2. The latter estimation rate is known to be optimal in many other nonparametric estimation problems, see for example [Tsybakov \(2008\)](#). It can also be remarked that, in both polynomial and exponential cases, the rates we get are very similar to the minimax rates obtained by [Brunel et al. \(2016, Theorem 4\)](#) or [Cardot and Johannes \(2010, Proposition 3.1\)](#) in the functional linear model with scalar outputs.

Although minimax optimal if the projection dimensions m_1 and m_2 are well chosen, the projection estimates are not adaptive at this stage. Indeed, the optimal dimension m_1 depends on the regularity α of the operator $S\Gamma^{1/2}$, which is generally unknown. In the next section, we focus on the construction of an adaptive estimator of the model, meaning that it does not imply any knowledge of the unknown model regularity and achieves the optimal required estimation rate.

4 Adaptive estimation

4.1 Model selection

The objective is to perform adaptive model selection, which does not depend on the unknown smoothness of the model S , but only on the available data. As a reminder, for given projection dimensions m_1 and m_2 , we estimate the operator S by $\widehat{S}_{m_1, m_2} = \widehat{\Pi}_{m_2} \Delta_n \Gamma_{n, m_1}^\dagger$, where the operators $\widehat{\Pi}_{m_2}$, Δ_n and Γ_{n, m_1}^\dagger are defined in Section 2.2.

The idea is to propose a procedure which automatically selects the best projection dimensions m_1 and m_2 , that is the best estimator in the collection $(\widehat{S}_{m_1, m_2})_{m_1, m_2}$. According to the result of Corollary 1, we choose $m_2 \rightarrow +\infty$ and we select m_1 in a collection $\mathcal{M}_n = \{1, \dots, N_n\}$, where the size of the collection N_n satisfied $N_n \leq \lfloor n/\ln^2(n) \rfloor$ where $\lfloor \cdot \rfloor$ is the floor function, associating to each x in \mathbb{R} the largest integer less or equal to x . Thus, the issue we consider now is the choice of an estimator in the collection $(\widehat{S}_{m_1, \infty})_{m_1 \in \mathcal{M}_n}$, where $\widehat{S}_{m_1, \infty} = \Delta_n \Gamma_{n, m_1}^\dagger$ corresponds in fact to the estimator of Crambes and Mas (2013). The method we use is derived from the model selection tools developed by Barron et al. (1999), as in Brunel et al. (2016) or Comte and Johannes (2012). A clear and detailed account is given in Massart (2007). We want to select the "best" estimator in the collection $(\widehat{S}_{m_1, \infty})_{m_1 \in \mathcal{M}_n}$, that is the one which has the smaller risk. Since the risk is unknown in practice, the oracle $m_1^* = \arg \min_{m_1 \in \mathcal{M}_n} \text{MSPE}(\widehat{S}_{m_1, \infty})$ is also unknown, and the risk $\text{MSPE}(\widehat{S}_{m_1, \infty})$ should be replaced by an empirical counterpart. Since the contrast function is an empirical version of the risk, the first idea is to choose $\arg \min_{m_1 \in \mathcal{M}_n} \gamma_n(\widehat{S}_{m_1, \infty})$. However, since the contrast function decreases when m_1 grows, the choice of $\arg \min_{m_1 \in \mathcal{M}_n} \gamma_n(\widehat{S}_{m_1, \infty})$ will lead to the selection of the largest index in the collection \mathcal{M}_n . One of the main idea of model selection theory is to introduce a penalty to balance this decrease, usually of the order of the variance. The dimension parameter m_1 is chosen as the one which minimizes a penalized contrast function,

$$\widehat{m}_1 = \arg \min_{m_1 \in \mathcal{M}_n} \left(\gamma_n(\widehat{S}_{m_1, \infty}) + \text{pen}(m_1) \right), \quad (12)$$

where γ_n is defined in Section 2.2 and pen is the penalty function defined as $\text{pen} : m_1 \mapsto 8(1+\delta)\sigma_\varepsilon^2 m_1/n$, with $\delta > 0$ a numerical constant that will be tuned in practice, see Section 5.

Remark that, when m_1 is fixed, $\gamma_n(\widehat{S}_{m_1, m_2})$ decreases with m_2 by definition and $\text{pen}(m_1)$ does not depend on m_2 . Thus, $(\widehat{m}_1, +\infty)$ is also a solution of the minimization problem

$$\min_{(m_1, m_2) \in \mathcal{M}_n \times \mathbb{N} \setminus \{0\} \cup \{+\infty\}} \left(\gamma_n(\widehat{S}_{m_1, m_2}) + \text{pen}(m_1) \right).$$

With this writing, the selection procedure has strong similarities with the usual model selection procedures when two dimensions have to be selected (see e.g. Plancade 2013; Lacour 2007). Here, the specificity is that the penalty criterion does not depend on m_2 (since the variance term only depends on m_1). This makes it possible to consider, in an equivalent way, the criterion (12) we have defined, which focuses on m_1 only.

4.2 Oracle-type inequality

Theorem 3 proves that the penalty term introduced above has the good order of magnitude to automatically realize the best bias-variance trade-off. In the statement of the result, and in the sequel, $\|\cdot\|_n$ is the empirical norm defined for all operator T as $\|T\|_n^2 = 1/n \sum_{i=1}^n \|T(X_i)\|^2$ and $\widehat{\Pi}_{m_1, \infty}^{op}$ is the orthogonal projection onto the closure of $V_{m_1, \infty} = \text{Span}\{\widehat{\varphi}_k \otimes \widehat{\varphi}_j, 1 \leq j \leq m_1, m_2 \geq 1\}$. The proof can be found in Section 6.4.

Theorem 3. *Under Assumption \mathcal{A}_7 , we have the following upper bounding, for all $\zeta > 0$,*

$$\mathbb{E}\|S - \widehat{S}_{m_1, \infty}\|_n^2 \leq (1 + \zeta) \inf_{m_1 \in \mathcal{M}_n} \left\{ \mathbb{E}\|S - \widehat{\Pi}_{m_1, \infty}^{op} S\|_n^2 + c(\zeta) \text{pen}(m_1) \right\} + \frac{C'}{n},$$

for a constant $C' > 0$ which does not depend neither on n , nor on m_1 and $c(\zeta) = (2 + \zeta)/(1 + \zeta)$.

Theorem 3 proves that the selected estimator achieves the best bias-variance compromise, up to a multiplicative constant, and the addition of the term C'/n , which is negligible. Then it achieves the minimax rate and, since the dimension selection procedure does not require the knowledge of the unknown regularity α , it is adaptive. A similar result could be obtained for the risk MSPE, but at the price of additional technicalities. Indeed, to obtain such result it is necessary to prove that, with sufficiently large probability, the quantity $\|S\|_n^2/\text{MSPE}(S)$ is lower bounded by a constant, for all $S \in V_{m_1, m_2}$ which is a random space (depending on the data X_1, \dots, X_n). We could draw inspiration e.g. from the proof of Brunel et al. (2016, Lemma 6).

5 Numerical study

The aim of this section is to assess the performance of the adaptive estimation method presented in Section 4. In Section 5.1, we perform simulation studies for various functional models. Subsequently, we apply the estimation method on two real data cases, in Section 5.2. All the study has been carried out with the free software R.

5.1 Simulation study

5.1.1 Simulated data

To implement our estimation method, we consider three data generating mechanisms (i), (ii) and (iii). Each model is defined by the equation

$$Y^{(\ell)} = \int_0^1 \mathcal{S}_\ell(s, \cdot) X^{(\ell)}(s) ds + \varepsilon^{(\ell)}, \quad (13)$$

where $\ell = 1, 2, 3$. We also denote $S^{(\ell)}$ the integral operator with kernel \mathcal{S}_ℓ . The analytical expressions of the kernels and noises are given below.

- (i) The kernel is defined as $\mathcal{S}_1 : (s, t) \mapsto s^2 + t^2$ and the noise $\varepsilon^{(1)}$ is generated according to a standard Brownian motion divided by 20. In addition, the Karhunen–Loève decomposition of the covariate $X^{(1)}$ is written as $X^{(1)} = \sum_{j=1}^{k_0} \sqrt{\lambda_j} \xi_j \varphi_j$, where $k_0 = 8$, $\lambda_j = 1/(\pi^2(j - 0.5)^2)$, $\varphi_j : t \mapsto \sqrt{2} \sin((j - 0.5)\pi t)$, $j = 1, \dots, k_0$, and $(\xi_j)_j$ are independent standard Gaussian random variables.
- (ii) The implementation of this simulation case is the same as (i) with only one difference, the error $\varepsilon^{(2)}$ is a Brownian motion divided by 2.
- (iii) The model kernel is given by the equation $\mathcal{S}_3 : (s, t) \mapsto \sum_{j,l=1}^{k_1} b_{j,l} \varphi_l(s) \varphi_j(t)$, where $k_1 = 50$, for all j, l in $\mathbb{N} \setminus \{0\}$, $\varphi_j : u \mapsto \sqrt{2} \cos(j\pi u)$ and $b_{j,l} = 4(-1)^{j+l} j^{-\gamma} l^{-\beta}$, with $\beta = 3$ and $\gamma = 2.5$. The input is the random function $X^{(3)} = \sum_{j=1}^{k_1} j^{-\alpha/2} U_j \varphi_j$, where $\alpha = 1.2$ and U_j are independent uniform distributions over $[-\sqrt{3}, \sqrt{3}]$. Finally, the noise is defined as $\varepsilon^{(3)} = \sum_{j=1}^{k_1} j^{-\delta/2} \xi_j \varphi_j$, with $\delta = 1.1$ and $(\xi_j)_{j \geq 1}$ are independent standard Gaussian random variables.

The simulation cases (i) and (ii) are drawn from Crambes and Mas (2013), while the model (iii) is studied in Imaizumi and Kato (2018) with slight modifications.

5.1.2 Implementation of the method

To perform the model selection strategy for the examples described above, a first step is to compute the penalty term of the procedure in (12). For simulation purposes, we keep the true value of σ_ε (it will be replaced by an empirical counterpart for real data analysis in Section 5.2). But we have to wisely choose the calibration parameter $\kappa = 8(1 + \delta)$, according to Section 4 notations. Unlike the theoretical framework and for practical reasons, the chosen values of κ are not necessarily greater than 8, as it is usual in model selection. More precisely, we compare the choices of κ values in the range $[0.2, 2]$, with a step of 0.2 between each two successive values. For every κ value and for each model, we generate $N = 500$ independent samples of inputs/outputs $(X_i, Y_i)_{i \in \{1, \dots, n\}}$ of size $n = 600$ each. We estimate the three models N times and for each iteration, we measure the prediction error by generating a new observation of the input/output pair. Thus, for any value of κ , and any $\ell = 1, 2, 3$, we simulate $(X_{i,k}^{(\ell)}, Y_{i,k}^{(\ell)})$ for $i = 1, \dots, n, k = 1, \dots, N$ from Model (13), we compute the Empirical Mean Square Prediction error

$$\text{EMSPE}^{(\ell, \kappa)} = \frac{1}{N} \sum_{k=1}^N \left\| \widehat{S}_{m_1, \infty}^{(\ell, \kappa)}(X_{n+1, k}^{(\ell)}) - S^{(\ell)}(X_{n+1, k}^{(\ell)}) \right\|^2$$

where $\widehat{S}_{m_1, \infty}^{(\ell, \kappa)}$ is the penalized contrast estimator computed from $(X_{i,k}^{(\ell)}, Y_{i,k}^{(\ell)})_{i=1, \dots, n}$ and $X_{n+1, k}^{(\ell)}$ is distributed like $X^{(\ell)}$ and independent of the $(X_{i,k}^{(\ell)})_i$.

Note also that numerically, we discretize the input X_i (respectively the output Y_i) realizations on a $[0, 1]$ uniform grid of size p (respectively q). The sizes of the grids are chosen to be $p = q = 100$. Figure 1 represents the Empirical Mean Square Prediction Error with respect to κ value, while Figure 2 shows the mean optimal selected dimension for each κ choice. A first general observation of curve shapes in Figure 1 is a tendency of decrease then increase. This reflects the fact that it is not recommended to choose neither too small nor too big calibration parameters. Indeed, small values favor the contrast term, while big values give the advantage to the penalty term, and in both cases the bias/variance compromise is missed. Another intuitive comment when comparing (i) and (ii) curves in Figure 1 is that the Empirical Mean Square Prediction Error of the second model is much bigger than the first one, which is consistent with the fact that the only difference between these models is that the second one is too noisy compared to the first one. Similar arguments can be used in the comparison of the Mean Prediction Error of the model (iii) with the two other ones. It is also worthwhile to point out that the optimal value is not necessarily unique, which can be suggested by the curve of (iii) in Figure 1. Moreover, the exact numerical values of the optimal parameters for the three models are respectively 0.6, 1.8 and 0.6. In the sequel, κ is set to the value 0.6. Furthermore, a simple overview of the graphics shows a systematic decrease of the Mean Optimal Dimension with respect to κ . This is due to the fact that high κ values amplify the penalty, which induce small selected dimensions. Also, by comparison of (i) and (ii) curves, the selected dimensions for the last model are much smaller than the first one. This is also a result of the noise variance magnitude. The numerical values of the Mean Optimal Dimension in the three cases are respectively 7.482, 2.886 and 39.95.

5.1.3 Simulation results

Now, we focus on the dispersion of the estimated prediction errors for different sample sizes. To do so, we consider three sample sizes $n = 200, 400, 600$ and we re-estimate $N = 500$ times the prediction errors for each model and n value. As mentioned before, κ is set to the value 0.6. The boxplots corresponding to each model are represented in Figure 3. As expected, as the sample sizes increase, the boxplots become tighter, the mean prediction errors get closer to zero and the outlier values decrease. This shows an improvement of the estimation accuracy with respect to the sample size, as expected. It is also noticeable that for equal sample sizes, the boxplots of the three models have the same form and a similar distribution of the outliers. This seems to suggest that the prediction quality is robust to the choice of the model and the noise magnitude.

To illustrate the prediction quality of the proposed adaptive estimators, we assume that for each model (i), (ii), and (iii), an input/output sample $(X_i^{(\ell)}, Y_i^{(\ell)})_{i=1, \dots, n}$ of size $n = 600$ is available ($\ell = 1, 2, 3$). These samples are used to estimate the operators S_ℓ , $\ell = 1, 2, 3$ and we predict the model output for 10 new independent inputs, denoted $X_{n+1}^{(\ell)}, \dots, X_{n+10}^{(\ell)}$. Figure 4 shows the obtained graphs for $S_\ell(X_{n+j}^{(\ell)})$ and

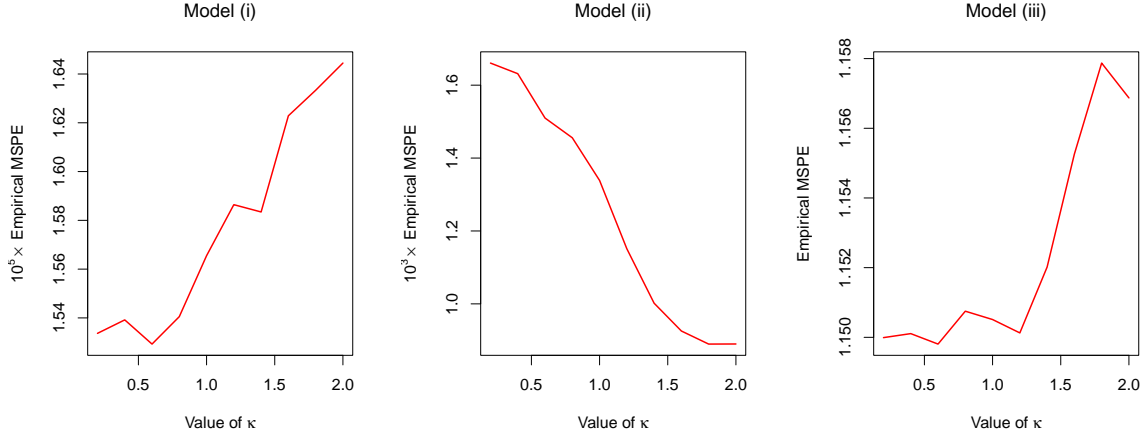


Figure 1: Empirical Mean Square Prediction Error (EMSPE) with respect to κ values for the models (i), (ii) and (iii).

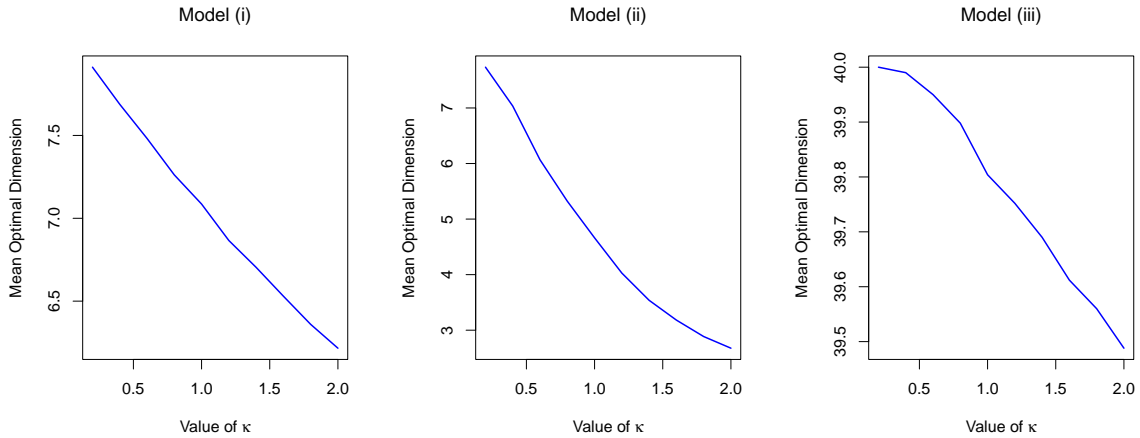


Figure 2: Mean Optimal Dimension with respect to κ values for the models (i), (ii) and (iii).

$\widehat{S}_\ell(X_{n+j}^{(\ell)})$, with $\ell = 1, 2, 3$ and $j = 1, \dots, 10$, while S_ℓ, \widehat{S}_ℓ respectively denote the real and estimated slope operators. In general, the prediction is quite accurate. Once again, a large noise magnitude deteriorates the prediction quality, which can be observed by comparing the graphs of the first two models.

5.2 Real data case

5.2.1 Application to the prediction of electricity consumption

The data we study are the electricity consumption of appliances curve of a low energy house located in Stambruge (Belgium). The dataset is freely available on UCI Machine Learning Repository <https://archive.ics.uci.edu/> and has been studied by Candanedo et al. (2017). It consists on measurements on 24 variables every 10 minutes from 11th january, 2016, 5pm to 27th may, 2016, 6pm. The variable of interest is the consumption of appliances, which is the main source of energy consumption. The data consists of a d -dimensional times series, with $d = 24$. It is first transformed into a sample of functional data by splitting the data day by day. We can deduce from the variable selection study conducted in Roche (2021) that the most important variable to predict appliances electricity consumption of day i is the appliances electricity consumption of day $i - 1$, and that a \ln -transformation of the covariates seems to lead to better results. Then, in our study, the variable to predict Y_i is the log of the appliances energy

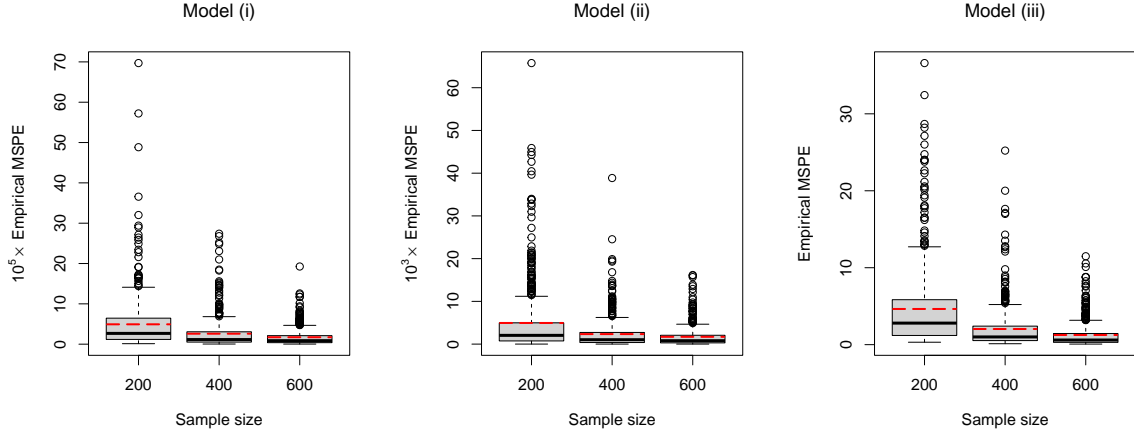


Figure 3: Boxplots of the Mean Square Prediction Errors for the models (i), (ii) and (iii) for $\kappa = 0.6$. The mean values are represented in red dashed lines.

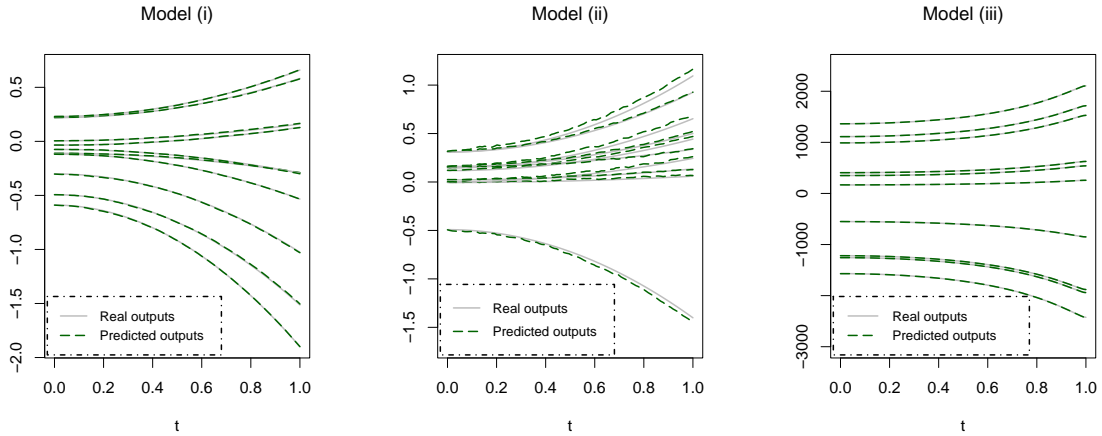


Figure 4: Prediction results : plots of $S^{(\ell)}(X_{n+j}^{(\ell)})$ (plain green lines) versus $\widehat{S}^{(\ell)}(X_{n+j}^{(\ell)})$ (dashed black lines) for $\ell = 1, 2, 3$, $j = 1, \dots, 10$, and where \widehat{S}_ℓ is computed from a sample of size $n = 600$.

consumption of day i and X_i is the log of appliances energy consumption of day $i - 1$. The data are also recentered. We present in Figure 5 the original and transformed data.

The incorporation of other functional covariates could be of great interest for the application but is out of the scope of the paper.

Another difficulty for the estimation procedure is that it requires the knowledge of the trace of the noise operator σ_ε^2 , which is unknown in practice. To get around this difficulty, we adapt the method proposed in Brunel et al. (2016), consisting in replacing the unknown quantity σ_ε^2 in criterion (12) by the contrast $\gamma_n(\widehat{S}_{m_1, \infty})$. In model selection in regression contexts, this method shows strong similarities with the one of Baraud et al. (2014). In the context of the functional linear model with scalar output, it has been proven in Brunel et al. (2016) that the estimator selected by this fully data-driven criterion verifies an oracle-type inequality, achieves the same minimax rates as the estimator selected by the criterion depending on the noise variance and that it does not change significantly the practical performances of the estimator.

As suggested by the simulation study, the value of κ is also fixed to $\kappa = 0.6$. To study the selected dimension, the risk of the estimators and their stability, we perform cross-validation of the sample: for each day i , we calculate the selected dimension $\widehat{m}_1^{(-i)}$ and the L^2 -prediction error of the estimator

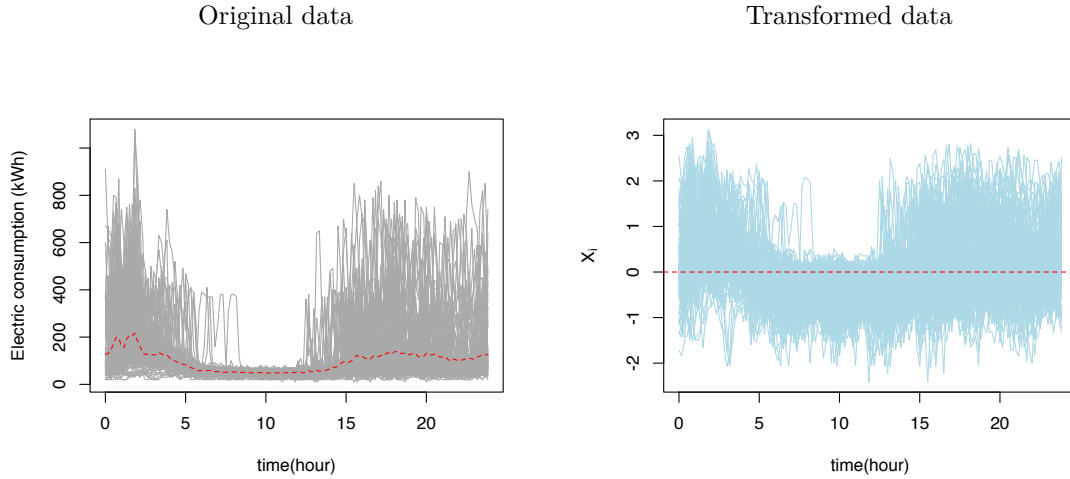


Figure 5: Evolution of electric consumption of appliances during $n = 136$ days (original data, thin gray lines) and functions of the sample (transformed data : centered version of the logarithm of the original data, thin blue lines). The dashed red lines are the empirical mean of each sample.

$\widehat{S}_{\widehat{m}_1^{(-i)}, \infty}^{-i}$ calculated from the sample $\{(X_j, Y_j), j \neq i\}$. The results are presented in Figure 6. The dimension selection procedure is quite stable, selecting more than 80% of time the dimension $\widehat{m}_1 = 11$ and the L^2 -prediction error does not explode for some observations.

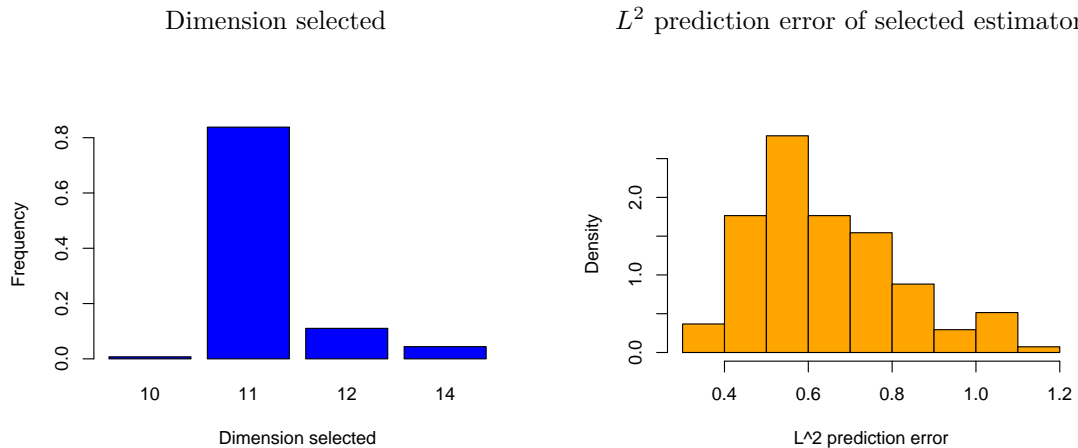


Figure 6: Dimension selected and L^2 prediction error $\|Y_i - \widehat{Y}_i^{(-i)}\|$ of the estimator calculated from each cross-validated sample.

We also plot in Figure 7, for three well-chosen days i ($i = 104$ is the day for which the distance $\|Y_i - \widehat{Y}_i^{(-i)}\|$ is minimal, $i = 4$ corresponds to the median prediction error and $i = 83$ to the maximal prediction error), the true value of Y_i and its prediction $\widehat{Y}_i^{(-i)} = \widehat{S}_{\widehat{m}_1^{(-i)}, \infty}^{-i}(X_i)$.

Figure 8 represents, for the same days, the prediction of appliances energy consumption (after adding the mean and taking the exponential).

We see in Figure 8 that prediction captures trends well and that the worst prediction seems to be due to a brutal change of behavior of the appliances electricity consumption which is quite hard to predict and may be due to external factors (hence unavoidable with our model).

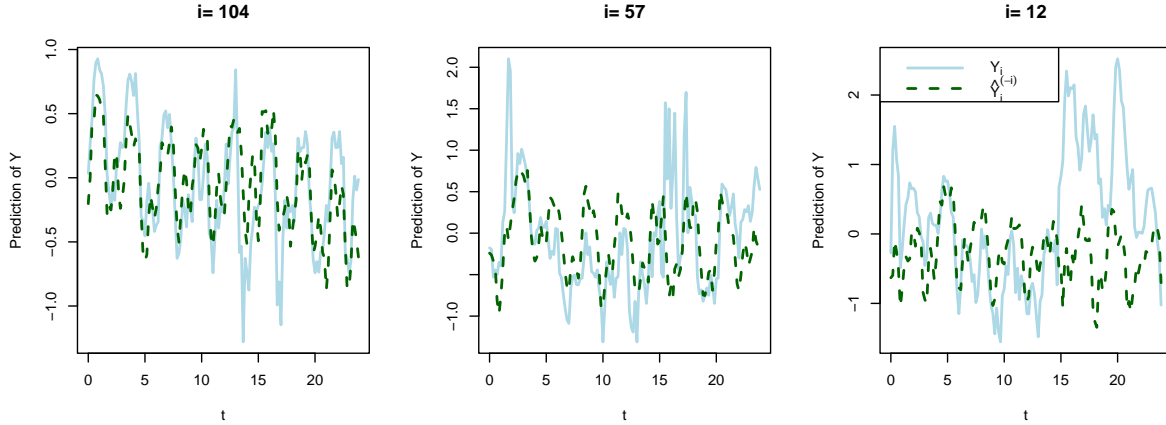


Figure 7: Cross-validated prediction \hat{Y}_i^{-i} made for three days (the days where the prediction is best, median and worst).

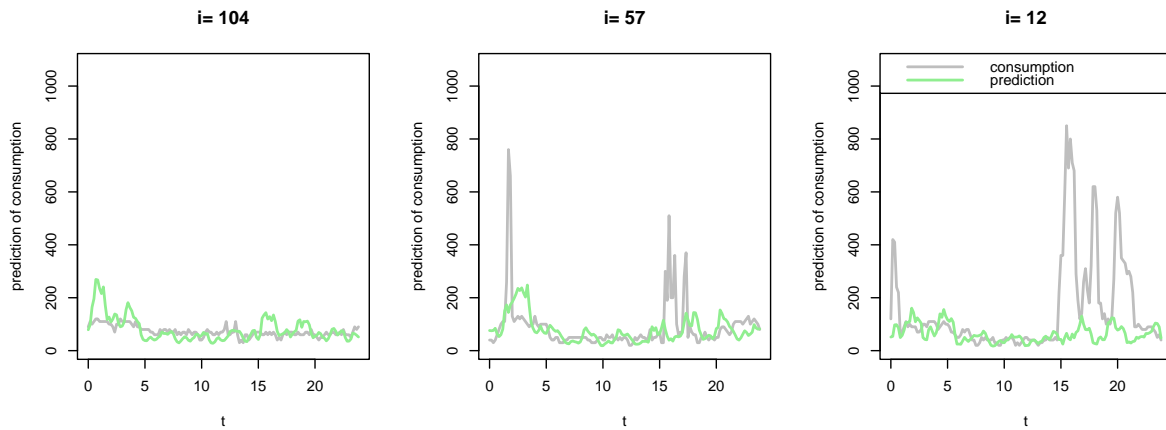


Figure 8: Prediction of appliances energy consumption.

5.2.2 Application to the prediction of prices from wind power infeed

We also apply now our estimation method to another, and more difficult prediction problem. The aim here is to predict the evolution of electricity prices in Germany from the wind power in-feed. This dataset has been extensively studied by [Liebl \(2013\)](#); [Imaizumi and Kato \(2018\)](#) and can be found at <https://www.dliebl.com/#publications>. We first remark that some observations exhibit non standard behaviors, in particular some prices are particularly elevated. Then, we start by removing the outliers that deserves a particular study which is out the scope of the paper. We consider a day to be an outlier if the maximal value of the price of the day is larger than $Q_3 + 1.5(Q_3 - Q_1)$ where Q_1 (resp. Q_3) corresponds to the first (resp. third) quartile of the maximal prices of each day. Then the data are also centered. We present in [Figure 9](#) the original and transformed data.

As in the previous section, we set $\kappa = 0.6$ and replace the unknown quantity σ_ε^2 by $\gamma_n(\hat{S}_{m_1, \infty})$. We also performed a cross-validation of selected dimensions and associated prediction risk. The results are presented in [Figure 10](#).

We also plot in [Figure 11](#), for three well-chosen days i the true value of Y_i and its prediction $\hat{Y}_i^{-i} = \hat{S}_{\hat{m}_1^{(-i)}, \infty}^{-i}(X_i)$: $i = 133$ is the day for which the distance $\|Y_i - \hat{Y}_i^{-i}\|$ is minimal, $i = 379$ corresponds to the median prediction error and $i = 43$ to the maximal prediction error.

Similarly to what happen in the previous real data problem (see [Figure 8](#) above), we see in [Figure 12](#)

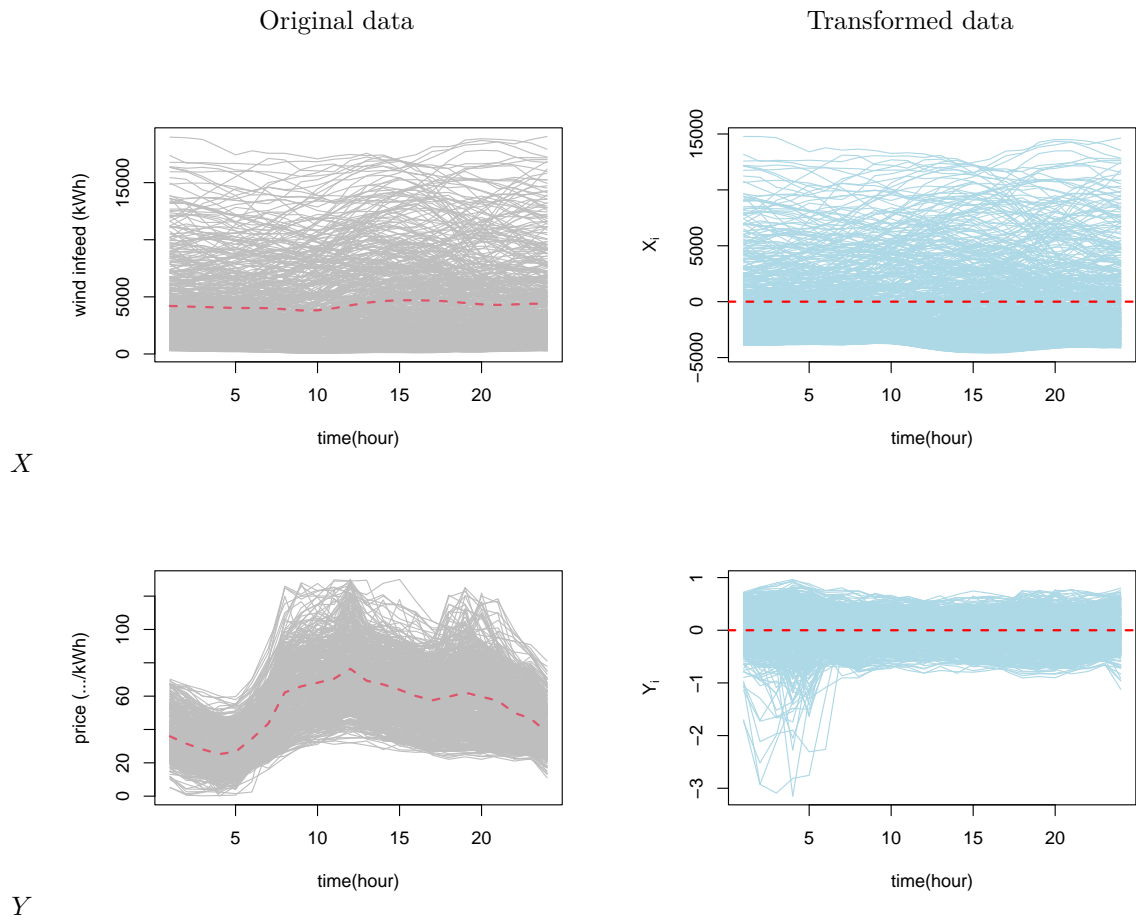


Figure 9: First line: evolution of wind power in-feed during $n = 516$ days (original data, thin gray lines) and functions of the sample (transformed data : centered version of the original data, thin blue lines). Second line: evolution of prices (original data, thin gray lines) and functions of the sample (transformed data : centered version of the log the original data+1, thin blue lines). The dashed red lines are the empirical mean of each sample.

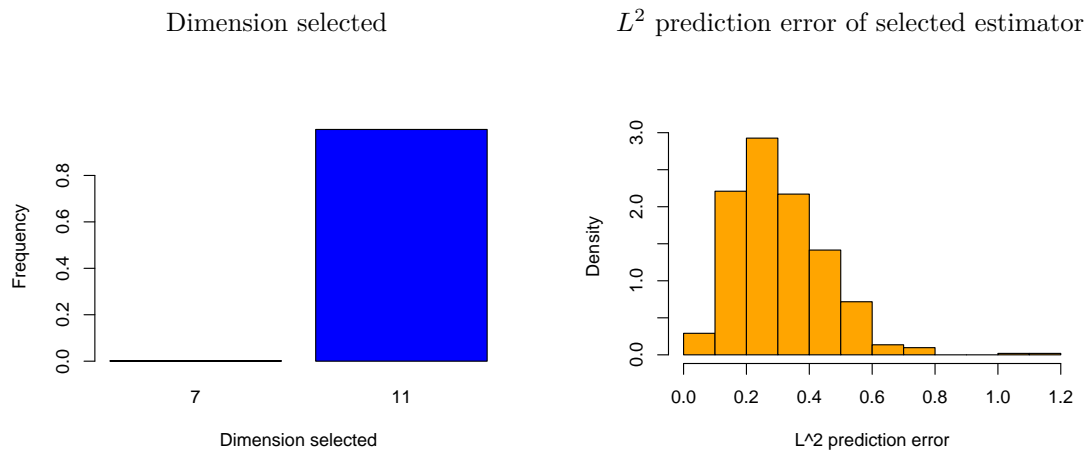


Figure 10: Dimension selected and L^2 prediction error $\|Y_i - \hat{Y}_i^{(-i)}\|$ of the estimator calculated from each cross-validated sample.

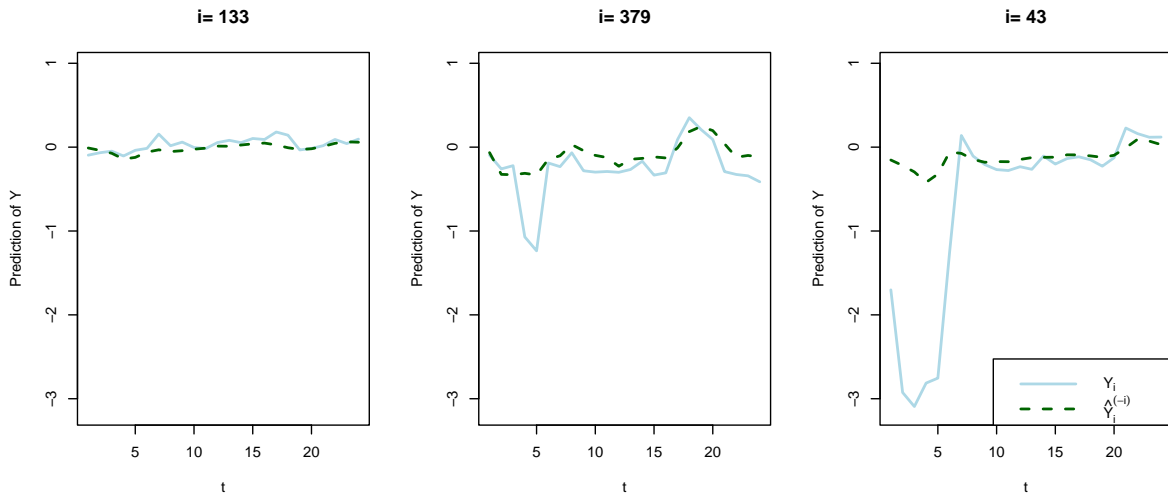


Figure 11: Cross-validated prediction \hat{Y}_i^{-i} made for three days.

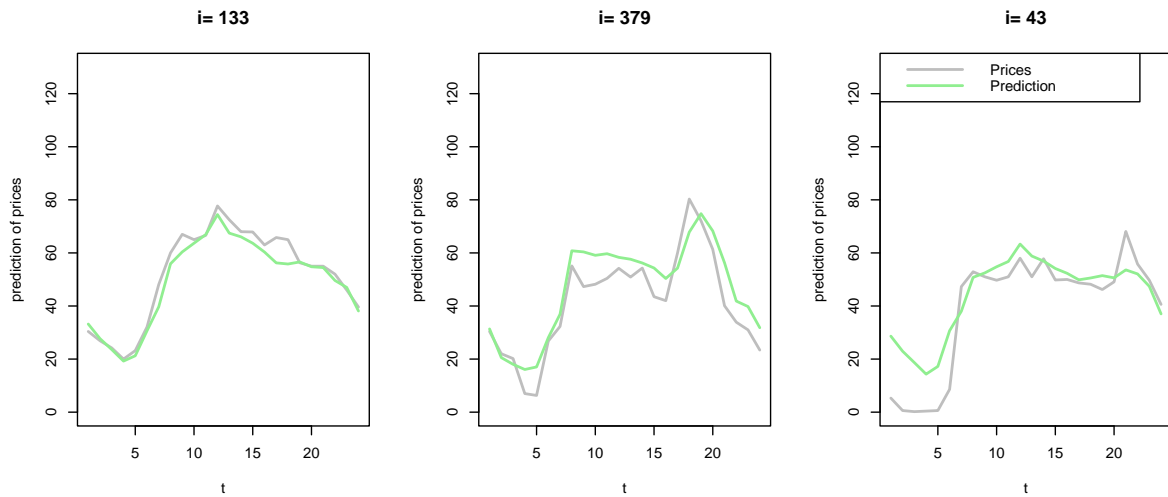


Figure 12: Cross-validated prediction \hat{Y}_i^{-i} made for three days taken randomly in the initial sample.

that the trends of each day is well captured and that the difficulty remains to predict the prices when there are brutal changes of behavior in the curves.

6 Proofs

All along the proofs, we denote by C a positive constant which does not depend on S , n or m and whose value may change from line to line. Many proofs are based on technical results from the perturbation theory of bounded operators. A short account of the preliminary results we need is given in Section 6.2 below. For more details, the reader can refer to [Dunford and Schwartz \(1965\)](#) and [Kato \(2013\)](#).

6.1 Proof of the results of Section 2

6.1.1 Proof of Proposition 1

The remark following Proposition 1 implies that it is equivalent to reason either on γ_n , or on γ'_n . We choose γ'_n . We have

$$\arg \min_{\mathcal{T} \in V'_{m_1, m_2}} \gamma'_n(\mathcal{T}) = \arg \min_{\mathcal{T} \in V'_{m_1, m_2}} \gamma'_{n,1}(\mathcal{T}) + \arg \min_{\mathcal{T} \in V'_{m_1, m_2}} \gamma'_{n,2}(\mathcal{T}),$$

where for any $\mathcal{T} \in V'_{m_1, m_2}$,

$$\gamma'_{n,1}(\mathcal{T}) = \frac{1}{n} \sum_{i=1}^n \left\| \int_0^1 \mathcal{T}(s, \cdot) X_i(s) ds \right\|^2, \quad \gamma'_{n,2}(\mathcal{T}) = -\frac{2}{n} \sum_{i=1}^n \langle Y_i, \int_0^1 \mathcal{T}(s, \cdot) X_i(s) ds \rangle.$$

For any $\mathcal{T} \in V'_{m_1, m_2}$, there also exists a unique sequence $b = (b_{j,k})_{j=1, \dots, m_1, k=1, \dots, m_2} \in \mathbb{R}^{m_1 m_2}$ such that

$$\mathcal{T}(s, t) = \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} b_{j,k} \phi_j(s) \phi_k(t),$$

with $(s, t) \in [0, 1]^2$. Thus,

$$\min_{\mathcal{T} \in V'_{m_1, m_2}} \gamma'_n(\mathcal{T}) = \min_{b \in \mathbb{R}^{m_1 m_2}} \tilde{\gamma}_n(b) \text{ with } \tilde{\gamma}'_n = \tilde{\gamma}'_{n,1} + \tilde{\gamma}'_{n,2},$$

and

$$\tilde{\gamma}'_{n,1}(b) = \frac{1}{n} \sum_{i=1}^n \sum_{k=1}^{m_2} \left(\sum_{j=1}^{m_1} b_{j,k} \langle \phi_j, X_i \rangle \right)^2, \quad \tilde{\gamma}'_{n,2}(b) = -\frac{2}{n} \sum_{i=1}^n \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} b_{j,k} \langle \phi_j, X_i \rangle \langle Y_i, \phi_k \rangle.$$

Thus, we look for a minimum of the function $\tilde{\gamma}_n$. The functions $\tilde{\gamma}_{n,\ell}$, $\ell = 1, 2$, are differentiable and for any $(j_0, k_0) \in \{1, \dots, m_1\} \times \{1, \dots, m_2\}$,

$$\frac{\partial \tilde{\gamma}_{n,1}(b)}{\partial b_{j_0, k_0}} = 2 \sum_{j=1}^{m_1} b_{j, k_0} \langle \Gamma_n \phi_{j_0}, \phi_j \rangle, \quad \frac{\partial \tilde{\gamma}_{n,2}(b)}{\partial b_{j_0, k_0}} = -\langle \Delta_n \phi_{j_0}, \phi_{k_0} \rangle.$$

This leads to $\nabla(\tilde{\gamma})(b) = 2Ab - 2Y_\phi$, with $b = (b_{j,k})_{j,k} \in \mathbb{R}^{m_1 m_2}$. We have proved that $b = A^{-1}Y_\phi$ is a critical point. Moreover, the Hessian matrix can be computed as follows:

$$\frac{\partial^2 \tilde{\gamma}_n(b)}{\partial b_{\ell, r} \partial b_{j_0, k_0}} = \delta_{r, k_0} \langle \Gamma_n \phi_{j_0}, \phi_{k_0} \rangle,$$

where $\delta_{r, k_0} = 1$ only if $r = k_0$, $\delta_{r, k_0} = 0$ otherwise. By considering the indices $(j, k) \in \{1, \dots, m_1\} \times \{1, \dots, m_2\}$ of a vector $b \in \mathbb{R}^{m_1 m_2}$, in the order $b = (b_{1,1}, \dots, b_{m_1,1}, b_{1,2}, \dots, b_{m_1,2}, \dots, b_{m_1, m_2})$, we obtain that the Hessian matrix of $\tilde{\gamma}_n$ on b is a block diagonal matrix, with m_2 blocks equal to $2A$. Thus, its determinant is $2^{m_2} (\det(A))^{m_2}$. Since A is the Gram matrix of a symmetric bilinear form, if it is invertible, the critical point is a global minimum, which proves Proposition 1.

6.1.2 Proof of Equality (7)

For any $T \in \mathcal{L}_2(\mathbb{H})$,

$$\Pi_{m_1, m_2}^{op} T = \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} \langle T, \varphi_k \otimes \varphi_j \rangle_{HS} \varphi_k \otimes \varphi_j,$$

with $\langle \cdot, \cdot \rangle_{HS}$ the scalar product associated to the Hilbert-Schmidt norm. Then, for any $r \in \mathbb{N} \setminus \{0\}$,

$$\begin{aligned} \Pi_{m_1, m_2}^{op} T(\varphi_r) &= \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} \langle T, \varphi_k \otimes \varphi_j \rangle_{HS} \varphi_k \otimes \varphi_j(\varphi_r), \\ &= \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} \langle T, \varphi_k \otimes \varphi_j \rangle_{HS} \delta_{j,r} \varphi_k, \text{ since the basis is orthonormal,} \\ &= \delta_{r \leq m_1} \sum_{k=1}^{m_2} \langle T, \varphi_k \otimes \varphi_r \rangle_{HS} \varphi_k, \\ &= \delta_{r \leq m_1} \sum_{k=1}^{m_2} \sum_{\ell=1}^{\infty} \langle T \varphi_\ell, \varphi_k \otimes \varphi_r(\varphi_\ell) \rangle \varphi_k, \text{ by definition of the scalar product,} \\ &= \delta_{r \leq m_1} \sum_{k=1}^{m_2} \langle T \varphi_r, \varphi_k \rangle \varphi_k = \delta_{r \leq m_1} \sum_{k=1}^{m_2} \varphi_k \otimes \varphi_k(T \varphi_r) = \delta_{r \leq m_1} \Pi_{m_2} T(\varphi_r), \\ &= \Pi_{m_2} T \Pi_{m_1}(\varphi_r). \end{aligned}$$

This ends the proof.

6.1.3 Proof of Proposition 2

Let us start with the proof of (8). Considering the result of Proposition 1, we begin with the computation of the elements of the matrix A , when we consider the PCA basis. We write

$$\langle \Gamma_n \widehat{\varphi}_j, \widehat{\varphi}_k \rangle = \langle \widehat{\lambda}_j \widehat{\varphi}_j, \widehat{\varphi}_k \rangle = \delta_{j,k} \widehat{\lambda}_j,$$

with $\delta_{j,k} = 0$ if $j \neq k$, $\delta_{j,k} = 1$ otherwise. Thus, A is a diagonal matrix, and in this case, if $\widehat{\lambda}_j > 0$, for any $j = 1, \dots, m_1$, we obtain the existence and uniqueness of the least-squares estimator, since A^{-1} exists and is equal to the diagonal matrix with diagonal elements $\widehat{\lambda}_j^{-1}$. The coefficients of the estimators are

$$\widehat{b}_{j,k} = \frac{1}{\widehat{\lambda}_j} \langle \Delta_n \widehat{\varphi}_j, \widehat{\varphi}_k \rangle, \quad j \in \{1, \dots, m_1\}, \quad k \in \{1, \dots, m_2\}.$$

This ends the proof of (8).

To prove (9), we start from (6), and the previous expression for $\widehat{\mathcal{S}}_m$. We immediatly get

$$\begin{aligned} \widehat{\mathcal{S}}_{m_1, m_2} &= \sum_{j=1}^{m_1} \sum_{k=1}^{m_2} \frac{1}{\widehat{\lambda}_j} \langle \Delta_n \widehat{\varphi}_j, \widehat{\varphi}_k \rangle \widehat{\varphi}_k \otimes \widehat{\varphi}_j, \\ &= \sum_{j=1}^{m_1} \frac{1}{\widehat{\lambda}_j} \langle \Delta_n \widehat{\varphi}_j, \widehat{\varphi}_j \rangle \widehat{\varphi}_j \otimes \widehat{\varphi}_j + \sum_{\substack{1 \leq j \leq m_1 \\ 1 \leq k \leq m_2 \\ j \neq k}} \frac{1}{\widehat{\lambda}_j} \langle \Delta_n \widehat{\varphi}_j, \widehat{\varphi}_k \rangle \widehat{\varphi}_k \otimes \widehat{\varphi}_j. \end{aligned}$$

It remains to apply the following lemma to the operator $T = \Delta_n \Gamma_{n, m_1}^\dagger$ of the first part of the right-hand-side of the last equality, and to remark that $\Gamma_{n, m_1}^\dagger \widehat{\varphi}_j = 0$ as soon as $j \geq m$.

Lemma 1. *Let T be a linear operator of a separable Hilbert space $(\mathbb{H}, \langle \cdot, \cdot \rangle)$, self-adjoint and compact. Let $(e_j)_{j \geq 1}$ be an orthonormal basis of eigenvectors of T . Then,*

$$T = \sum_{j=1}^{\infty} \langle T e_j, e_j \rangle e_j \otimes e_j.$$

Proof of Lemma 1

For any Hilbertian basis $(e_j)_{j \geq 1}$, it is well known that any operator T can be written

$$T = \sum_{j,k=1}^{\infty} \langle T e_j, e_k \rangle e_k \otimes e_j.$$

Now, if the e_j 's are orthonormal eigenfunctions of T , there exist eigenvalues θ_j such that

$$\langle T e_j, e_k \rangle = \theta_j \langle e_j, e_k \rangle = \theta_j \delta_{j,k},$$

with $\delta_{j,k} = 1$ if $j = k$, $\delta_{j,k} = 0$ otherwise. This proves the result.

6.2 Perturbation theory background

We provide here a digest of some key results of the perturbation theory, which will be helpful within the proofs. These results are largely sourced from Roche (2014); Brunel et al. (2016); Mas and Ruyngaert (2015), but also from Crambes and Mas (2013) and Cardot et al. (2007). In a nutshell, the aim of the perturbation theory is to control the proximity between the eigenfunctions of Γ and those of the random operator Γ_n . We remind that the operator Π_m (resp. $\widehat{\Pi}_m$) stands for the orthonormal projector onto $\text{Span}(\varphi_1, \dots, \varphi_m)$ (resp. $\text{Span}(\widehat{\varphi}_1, \dots, \widehat{\varphi}_m)$).

Let us denote by \mathcal{B}_j the oriented circle of the complex plane of center λ_j and radius $\delta_j/2$, where $\delta_j = \lambda_j - \lambda_{j+1}$. We also define $\mathcal{C}_m = \bigcup_{j=1}^m \mathcal{B}_j$ which is a union of disjoint circles since, by Assumption \mathcal{A}_2 , we also have $\delta_j = \min\{\lambda_j - \lambda_{j+1}, \lambda_{j-1} - \lambda_j\}$. Let also $\mathbf{a}_j = \frac{\lambda_j}{\delta_j} + \sum_{r \neq j} \frac{\lambda_r}{|\lambda_r - \lambda_j|}$, for all $j \geq 1$, we define the set

$$\mathcal{A}_n = \bigcap_{j=1}^m \left\{ |\widehat{\lambda}_j - \lambda_j| < \frac{\delta_j}{2} \right\} \cap \left\{ \sup_{z \in \text{supp}(\mathcal{C}_m)} \|T_n(z)\|_{\infty} < \frac{\mathbf{a}_j}{\sqrt{n}} \ln(n) \right\}.$$

The following lemma is the keystone of the results related to perturbation theory. It provides a link between the difference of the empirical and theoretical projectors $\widehat{\Pi}_m - \Pi_m$, which we want to control, and the difference between empirical and theoretical covariance operators $\Gamma_n - \Gamma$, which can be controlled with the Bernstein inequality.

Lemma 2. *Under Assumption \mathcal{A}_5 , there exists a set \mathcal{A}_n such that*

$$\mathbb{P}(\mathcal{A}_n^c) \leq \exp(-c^* \ln(n)^2),$$

where c^* is some positive constant depending on $(\lambda_j)_{j \geq 1}$ and

$$(\widehat{\Pi}_m - \Pi_m) \mathbf{1}_{\mathcal{A}_n} = \frac{1}{2i\pi} \sum_{k=1}^m \int_{\mathcal{B}_k} R(z) (\Gamma_n - \Gamma) R(z) dz \mathbf{1}_{\mathcal{A}_n} + \frac{1}{2i\pi} \sum_{k=1}^m \int_{\mathcal{B}_k} R^{1/2}(z) [I - T_n(z)]^{-1} T_n(z)^2 R^{1/2}(z) dz \mathbf{1}_{\mathcal{A}_n},$$

with $T_n(z) = R^{1/2}(z) (\Gamma_n - \Gamma) R^{1/2}(z)$ and $R(z) = (zI - \Gamma)^{-1}$.

Lemma 2 is proved in Brunel et al. (2016) (see Lemma 12 and Remark 4, p.224).

Throughout the proofs, we will also need some results on the behavior of the eigenvalues $(\lambda_j)_{j \geq 1}$. Lemma 3 and Lemma 4 the main results we will need.

Lemma 3. (Cardot et al., 2007, Lemma 1) *Assume that Assumption \mathcal{A}_3 is satisfied. Then, for all positive integers j and k , such that $k > j$, we have*

$$j\lambda_j \geq k\lambda_k \quad \text{and} \quad \lambda_j - \lambda_k \geq \left(1 - \frac{j}{k}\right) \lambda_j.$$

In addition,

$$\sum_{r \geq k} \lambda_r \leq (k+1)\lambda_k.$$

Lemma 4. (Hilgert et al., 2013, Lemma 10.1) *Under Assumptions \mathcal{A}_4 and \mathcal{A}_6 , we have*

$$\mathbf{a}_k \leq Ck \ln(k).$$

6.3 Proofs of the results of Section 3

In order to achieve the bias-variance decomposition for the prediction risk presented in Section 3, we will need to formulate \widehat{S}_{m_1, m_2} in terms of S . We remind that

$$\widehat{S}_{m_1, m_2} = \widehat{\Pi}_{m_2} \Delta_n \Gamma_{n, m_1}^\dagger. \quad (14)$$

Due to the linearity of S , it is straightforward that

$$\Delta_n = S\Gamma_n + \frac{1}{n} \sum_{i=1}^n \varepsilon_i \otimes X_i.$$

Now, given that Γ_{n, m_1}^\dagger is self-adjoint, one can easily see that

$$\Delta_n \Gamma_{n, m_1}^\dagger = S\widehat{\Pi}_{m_1} + U_n, \quad (15)$$

where $U_n = n^{-1} \sum_{i=1}^n \varepsilon_i \otimes \Gamma_{n, m_1}^\dagger(X_i)$. Combining Equations (14) and (15) allows us to write

$$\widehat{S}_{m_1, m_2} = \widehat{\Pi}_{m_2} S\widehat{\Pi}_{m_1} + \widehat{\Pi}_{m_2} U_n. \quad (16)$$

Besides, Lemma 5 stated just below will be very helpful for onward proofs.

Lemma 5. *Let V and W be random bounded linear operators, independent of X_{n+1} . We assume that V and W are Hilbert-Schmidt operators. Then,*

$$\mathbb{E}\langle V(X_{n+1}), W(X_{n+1}) \rangle = \mathbb{E}\langle V\Gamma^{1/2}, W\Gamma^{1/2} \rangle_{\text{HS}},$$

where $\langle \cdot, \cdot \rangle_{\text{HS}}$ refers to the Hilbert-Schmidt scalar product and

$$\mathbb{E}\|V(X_{n+1})\|^2 = \mathbb{E}\|V\Gamma^{1/2}\|_{\text{HS}}^2.$$

Proof of Lemma 5. We start by

$$\begin{aligned} \mathbb{E}\langle V(X_{n+1}), W(X_{n+1}) \rangle &= \sum_{j=1}^{+\infty} \mathbb{E}\langle X_{n+1}, \varphi_j \rangle \langle V(\varphi_j), W(X_{n+1}) \rangle \\ &= \sum_{j=1}^{+\infty} \mathbb{E}\langle V(\varphi_j), W(\langle X_{n+1}, \varphi_j \rangle X_{n+1}) \rangle. \end{aligned}$$

From here, we first compute the expectation with respect to X_{n+1} . Given both the linearity of W and that X_{n+1} is independent of V and W , we obtain

$$\begin{aligned} \mathbb{E}\langle V(X_{n+1}), W(X_{n+1}) \rangle &= \sum_{j=1}^{+\infty} \mathbb{E}\langle V(\varphi_j), W\Gamma(\varphi_j) \rangle \\ &= \sum_{j=1}^{+\infty} \lambda_j \mathbb{E}\langle V(\varphi_j), W(\varphi_j) \rangle. \end{aligned}$$

Therefore,

$$\begin{aligned} \mathbb{E}\langle V(X_{n+1}), W(X_{n+1}) \rangle &= \sum_{j=1}^{+\infty} \mathbb{E}\langle V\Gamma^{1/2}(\varphi_j), W\Gamma^{1/2}(\varphi_j) \rangle \\ &= \mathbb{E}\langle V\Gamma^{1/2}, W\Gamma^{1/2} \rangle_{\text{HS}}. \end{aligned}$$

This proves the first equality of Lemma 5, and the second one is a direct consequence, taking $V = W$.

6.3.1 Proof of Theorem 1

The starting point of the proof is to achieve a first bias-variance decomposition of the prediction risk. As a result of Lemma 5, we note

$$\mathbb{E}\|\widehat{S}_{m_1, m_2}(X_{n+1}) - S(X_{n+1})\|^2 = \mathbb{E}\|(\widehat{S}_{m_1, m_2} - S)\Gamma^{1/2}\|_{\text{HS}}^2.$$

In addition, from Equation (16), we write

$$\begin{aligned} \mathbb{E}\|\widehat{S}_{m_1, m_2}(X_{n+1}) - S(X_{n+1})\|^2 &= \mathbb{E}\|(\widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1} - S)\Gamma^{1/2} + \widehat{\Pi}_{m_2} U_n \Gamma^{1/2}\|_{\text{HS}}^2 \\ &= \mathbb{E}\|(S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})\Gamma^{1/2}\|_{\text{HS}}^2 + \mathbb{E}\|\widehat{\Pi}_{m_2} U_n \Gamma^{1/2}\|_{\text{HS}}^2 \\ &\quad - 2\mathbb{E}\langle (S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})\Gamma^{1/2}, \widehat{\Pi}_{m_2} U_n \Gamma^{1/2} \rangle_{\text{HS}}. \end{aligned} \quad (17)$$

The last right-side expectation of Equation (17) is null. Indeed, recall that

$$\mathbb{E}\langle (S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})\Gamma^{1/2}, \widehat{\Pi}_{m_2} U_n \Gamma^{1/2} \rangle_{\text{HS}} = \sum_{j=1}^{+\infty} \lambda_j \mathbb{E}\langle (S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})(\varphi_j), \widehat{\Pi}_{m_2} U_n(\varphi_j) \rangle.$$

Notice that, $\widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1}$ only depends on (X_1, \dots, X_n) . It remains then to show that the expectation of $\widehat{\Pi}_{m_2} U_n(\varphi_j)$ conditionally to (X_1, \dots, X_n) is zero. We write,

$$\begin{aligned} \mathbb{E}[\widehat{\Pi}_{m_2} U_n(\varphi_j) | X_1, \dots, X_n] &= \frac{1}{n} \sum_{i=1}^n \mathbb{E}[\langle \Gamma_{n, m_1}^\dagger(X_i), \varphi_j \rangle \widehat{\Pi}_{m_2}(\varepsilon_i) | X_1, \dots, X_n] \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{r=1}^{m_2} \langle \Gamma_{n, m_1}^\dagger(X_i), \varphi_j \rangle \mathbb{E}[\langle \varepsilon_i, \varphi_r \rangle \varphi_r | X_1, \dots, X_n] \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{r=1}^{m_2} \langle \Gamma_{n, m_1}^\dagger(X_i), \varphi_j \rangle \langle \mathbb{E}[\varepsilon_i], \varphi_r \rangle \varphi_r \\ &= 0_{\mathbb{H}}. \end{aligned}$$

In other words,

$$\mathbb{E}\langle (S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})\Gamma^{1/2}, \widehat{\Pi}_{m_2} U_n \Gamma^{1/2} \rangle_{\text{HS}} = 0.$$

Therefore,

$$\mathbb{E}\|\widehat{S}_{m_1, m_2}(X_{n+1}) - S(X_{n+1})\|^2 = \mathbb{E}\|(S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})\Gamma^{1/2}\|_{\text{HS}}^2 + \mathbb{E}\|\widehat{\Pi}_{m_2} U_n \Gamma^{1/2}\|_{\text{HS}}^2. \quad (18)$$

In Equation (18), we recognize the common decomposition of the estimation risk as a compromise of a bias and variance terms. The bias, namely the first term in the right side, is decreasing with respect to m_1 and m_2 and is related to the regularity of the regression model S . While the variance term is increasing with respect to m_2 and depending in particular on the observation errors $\varepsilon_1, \dots, \varepsilon_n$. In the following propositions 3 and 4, we give sharp upper bounds of these two terms, which ends the proof.

Proposition 3. *The variance term of Equation (18) can be upper bounded as*

$$\mathbb{E}\|\widehat{\Pi}_{m_2} U_n \Gamma^{1/2}\|_{\text{HS}}^2 \leq \sigma_\varepsilon^2 \frac{m_1}{n} + A_{n, m_1},$$

where $\sigma_\varepsilon = \mathbb{E}\|\varepsilon\|^2$ and $A_{n, m_1} = \sigma_\varepsilon^2 \frac{C m_1^2 \ln^2(m_1)}{n^2}$.

Proposition 4. *The bias term of Equation (18) can be upper bounded as*

$$\mathbb{E}\|(S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1})\Gamma^{1/2}\|_{\text{HS}}^2 \leq 3 \sum_{j=m_1+1}^{+\infty} \lambda_j \|S(\varphi_j)\|^2 + 3 \sum_{j=1}^{m_1} \lambda_j \|(I - \Pi_{m_2})S(\varphi_j)\|^2 + B_{n, m_1} + D_{n, m_2} + E_n.$$

where

$$\begin{aligned} B_{n, m_1} &= \frac{C m_1^2 \lambda_{m_1} \|S\|_{\text{HS}}}{n}, \quad E_n = \frac{C}{n^2} \|\Sigma \Gamma^{1/2}\|_{\text{HS}}^2 \\ D_{n, m_2} &= \frac{C m_2 \lambda_{m_2}}{n} + \frac{C m_2^2 \ln(m_2)}{n \psi_\beta(m_2)} + \frac{C m_2^3}{n \psi_\beta(\lfloor m_2/2 \rfloor)} + \frac{C \ln^4(n)}{n^2} \left(\sum_{k=1}^{m_2} \frac{k^2 \ln^2(k)}{\sqrt{\psi_\beta(k)}} \right)^2. \end{aligned}$$

Proof of Proposition 3. It is obvious that

$$\begin{aligned}\mathbb{E}\|\widehat{\Pi}_{m_2}U_n\Gamma^{1/2}\|_{\text{HS}}^2 &= \sum_{j=1}^{+\infty}\sum_{r=1}^{m_2}\lambda_j\mathbb{E}\langle U_n(\varphi_j), \varphi_r \rangle^2 \\ &= \frac{1}{n^2}\sum_{j=1}^{+\infty}\sum_{r=1}^{m_2}\lambda_j\mathbb{E}\left[\sum_{i=1}^n\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle \langle \varepsilon_i, \varphi_r \rangle\right]^2.\end{aligned}$$

Then,

$$\begin{aligned}\mathbb{E}\|\widehat{\Pi}_{m_2}U_n\Gamma^{1/2}\|_{\text{HS}}^2 &= \frac{1}{n^2}\sum_{j=1}^{+\infty}\sum_{r=1}^{m_2}\sum_{i=1}^n\lambda_j\mathbb{E}\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle^2 \langle \varepsilon_i, \varphi_r \rangle^2 \\ &\quad + \frac{1}{n^2}\sum_{j=1}^{+\infty}\sum_{r=1}^{m_2}\sum_{\substack{i \neq i' \\ (i,i') \in [1,n]^2}}\lambda_j\mathbb{E}\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle \langle \Gamma_{n,m_1}^\dagger(X_{i'}), \varphi_j \rangle \langle \varepsilon_i, \varphi_r \rangle \langle \varepsilon_{i'}, \varphi_r \rangle.\end{aligned}$$

All the terms of the second right-side sum are null. Indeed, by independence of $(\varepsilon_1, \dots, \varepsilon_n)$ and (X_1, \dots, X_n) , we have for $i \neq i'$,

$$\begin{aligned}\mathbb{E}\left[\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle \langle \Gamma_{n,m_1}^\dagger(X_{i'}), \varphi_j \rangle \langle \varepsilon_i, \varphi_r \rangle \langle \varepsilon_{i'}, \varphi_r \rangle \mid X_1, \dots, X_n\right] \\ = \langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle \langle \Gamma_{n,m_1}^\dagger(X_{i'}), \varphi_j \rangle \mathbb{E}\left[\langle \varepsilon_i, \varphi_r \rangle \langle \varepsilon_{i'}, \varphi_r \rangle \mid X_1, \dots, X_n\right].\end{aligned}$$

Thus, knowing that $\varepsilon_1, \dots, \varepsilon_n$ are independent and centered, we have

$$\begin{aligned}\mathbb{E}\left[\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle \langle \Gamma_{n,m_1}^\dagger(X_{i'}), \varphi_j \rangle \langle \varepsilon_i, \varphi_r \rangle \langle \varepsilon_{i'}, \varphi_r \rangle \mid X_1, \dots, X_n\right] \\ = \langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle \langle \Gamma_{n,m_1}^\dagger(X_{i'}), \varphi_j \rangle \langle \mathbb{E}[\varepsilon_i], \varphi_r \rangle \langle \mathbb{E}[\varepsilon_{i'}], \varphi_r \rangle = 0.\end{aligned}$$

Therefore, the variance term is simply given by

$$\begin{aligned}\mathbb{E}\|\widehat{\Pi}_{m_2}U_n\Gamma^{1/2}\|_{\text{HS}}^2 &= \frac{1}{n^2}\sum_{i=1}^n\sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle^2 \mathbb{E}\|\Pi_{m_2}(\varepsilon_i)\|^2 \\ &\leq \frac{\sigma_\varepsilon^2}{n^2}\sum_{i=1}^n\sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle^2,\end{aligned}$$

where $\sigma_\varepsilon^2 = \mathbb{E}\|\varepsilon\|^2$. Furthermore, giving that Γ_{n,m_1}^\dagger is self-adjoint, we get

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^n\sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle \Gamma_{n,m_1}^\dagger(X_i), \varphi_j \rangle^2 &= \frac{1}{n}\sum_{i=1}^n\sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle X_i, \Gamma_{n,m_1}^\dagger(\varphi_j) \rangle^2 \\ &= \frac{1}{n}\sum_{i=1}^n\sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle \langle X_i, \Gamma_{n,m_1}^\dagger(\varphi_j) \rangle X_i, \Gamma_{n,m_1}^\dagger(\varphi_j) \rangle \\ &= \sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle \Gamma_n\Gamma_{n,m_1}^\dagger(\varphi_j), \Gamma_{n,m_1}^\dagger(\varphi_j) \rangle.\end{aligned}$$

Yet, it is easy to see that $\Gamma_{n,m_1}^\dagger\Gamma_n\Gamma_{n,m_1}^\dagger = \Gamma_{n,m_1}^\dagger\widehat{\Pi}_{m_1} = \Gamma_{n,m_1}^\dagger$. Thus,

$$\mathbb{E}\|\widehat{\Pi}_{m_2}U_n\Gamma^{1/2}\|_{\text{HS}}^2 \leq \frac{\sigma_\varepsilon^2}{n}\sum_{j=1}^{+\infty}\lambda_j\mathbb{E}\langle \Gamma_{n,m_1}^\dagger(\varphi_j), \varphi_j \rangle.$$

Now, it is fairly easy to show the following equation. This can be done by diagonalization of the self-adjoint operator Γ_{n,m_1}^\dagger in the orthonormal basis of its eigenfunctions, we write

$$\langle \Gamma_{n,m_1}^\dagger(\varphi_j), \varphi_j \rangle = \text{Tr}(\Gamma_{n,m_1}^\dagger \cdot \varphi_j \otimes \varphi_j),$$

where the notation \cdot refers to the Hadamard product for operators (i.e. for two operators $S, T \in \mathcal{L}(H)$, $S \cdot T = \sum_{j,k \geq 1} \langle S, \varphi_j \rangle \langle T, \varphi_k \rangle \varphi_j \otimes \varphi_k$). Then,

$$\begin{aligned} \mathbb{E} \|\widehat{\Pi}_{m_2} U_n \Gamma^{1/2}\|_{\text{HS}}^2 &\leq \frac{\sigma_\varepsilon^2}{n} \mathbb{E} [\text{Tr} (\Gamma_{n, m_1}^\dagger \cdot \Gamma)] \\ &= \frac{\sigma_\varepsilon^2}{n} [\text{Tr} (\mathbb{E} [(\Gamma_{n, m_1}^\dagger - \Gamma^\dagger) \cdot \Gamma]) + \text{Tr} (\Gamma^\dagger \cdot \Gamma)]. \end{aligned}$$

Moreover, based on [Crambes and Mas \(2013, Lemma 19\)](#), we have

$$\text{Tr} (\mathbb{E} [(\Gamma_{n, m_1}^\dagger - \Gamma^\dagger) \cdot \Gamma]) \leq \frac{Cm_1^2 \ln^2(m_1)}{n}.$$

At last, remark that $\text{Tr} (\Gamma^\dagger \cdot \Gamma) = \text{Tr} (\Pi_{m_1}) = m_1$, which finishes the proof.

Proof of Proposition 4. To achieve a sharp upper bound for the bias term, we intensively rely on the perturbation theory for bounded operators presented in [Section 6.2](#). We also use some results already established in [Crambes and Mas \(2013\)](#). We begin with the following plain decomposition,

$$S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1} = S - \Pi_{m_2} S \Pi_{m_1} - \widehat{\Pi}_{m_2} S (\widehat{\Pi}_{m_1} - \Pi_{m_1}) - (\widehat{\Pi}_{m_2} - \Pi_{m_2}) S \Pi_{m_1}.$$

Then,

$$\begin{aligned} \mathbb{E} \|(S - \widehat{\Pi}_{m_2} S \widehat{\Pi}_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 &\leq 3\mathbb{E} \|(S - \Pi_{m_2} S \Pi_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 + 3\mathbb{E} \|\widehat{\Pi}_{m_2} S (\widehat{\Pi}_{m_1} - \Pi_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 \\ &\quad + 3\mathbb{E} \|(\widehat{\Pi}_{m_2} - \Pi_{m_2}) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2. \end{aligned} \quad (19)$$

In the remainder of the proof, we upper bound each term of Equation (19). We have

$$\begin{aligned} \mathbb{E} \|(S - \Pi_{m_2} S \Pi_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 &= \mathbb{E} \|S(\mathbf{I} - \Pi_{m_1}) \Gamma^{1/2} + (\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 \\ &= \mathbb{E} \|S(\mathbf{I} - \Pi_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 + \mathbb{E} \|(\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 \\ &\quad + 2\mathbb{E} \langle S(\mathbf{I} - \Pi_{m_1}) \Gamma^{1/2}, (\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1} \Gamma^{1/2} \rangle_{\text{HS}}. \end{aligned}$$

The last right-side term of the equation just above is zero. Indeed,

$$\begin{aligned} \langle S(\mathbf{I} - \Pi_{m_1}) \Gamma^{1/2}, (\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1} \Gamma^{1/2} \rangle_{\text{HS}} &= \sum_{j=1}^{+\infty} \lambda_j \langle S(\mathbf{I} - \Pi_{m_1})(\varphi_j), (\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1}(\varphi_j) \rangle \\ &= 0. \end{aligned}$$

Besides,

$$\begin{aligned} \mathbb{E} \|S(\mathbf{I} - \Pi_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 &= \sum_{j=1}^{+\infty} \lambda_j \|S(\mathbf{I} - \Pi_{m_1})(\varphi_j)\|^2 \\ &= \sum_{j=m_1+1}^{+\infty} \lambda_j \|S(\varphi_j)\|^2. \end{aligned}$$

In addition,

$$\begin{aligned} \mathbb{E} \|(\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 &= \sum_{j=1}^{+\infty} \lambda_j \|(\mathbf{I} - \Pi_{m_2}) S \Pi_{m_1}(\varphi_j)\|^2 \\ &= \sum_{j=1}^{m_1} \lambda_j \|(\mathbf{I} - \Pi_{m_2}) S(\varphi_j)\|^2. \end{aligned}$$

This means that

$$\mathbb{E} \|(S - \Pi_{m_2} S \Pi_{m_1}) \Gamma^{1/2}\|_{\text{HS}}^2 = \sum_{j=m_1+1}^{+\infty} \lambda_j \|S(\varphi_j)\|^2 + \sum_{j=1}^{m_1} \lambda_j \|(\mathbf{I} - \Pi_{m_2}) S(\varphi_j)\|^2. \quad (20)$$

We now upper bound the second right-side term of Equation (19). It is easy to see that

$$\mathbb{E}\|\widehat{\Pi}_{m_2}S(\widehat{\Pi}_{m_1} - \Pi_{m_1})\Gamma^{1/2}\|_{\text{HS}}^2 \leq \mathbb{E}\|S(\widehat{\Pi}_{m_1} - \Pi_{m_1})\Gamma^{1/2}\|_{\text{HS}}^2.$$

An upper bound of the right expectation in the previous equation is given in [Crambes and Mas \(2013, Proposition 15\)](#). However, we believe that following the article notations, a 'k' is missing in the upper bound. This happens on the page 2644, in the equation block below Formula (17), while switching from the second to the third equation. We would like to point out that this error does not alter the optimality of the results demonstrated in the paper, but it constrains the regularity of X . We also believe that thanks to Assumption \mathcal{A}_6 , this loss can be avoided. This make it possible to replace the square of the sum by the sum of squares. We then obtain,

$$\mathbb{E}\|\widehat{\Pi}_{m_2}S(\widehat{\Pi}_{m_1} - \Pi_{m_1})\Gamma^{1/2}\|_{\text{HS}}^2 \leq \frac{Cm_1^2\lambda_{m_1}\|S\|_{\text{HS}}}{n}. \quad (21)$$

Upper-bounding the last term of (19) requires a wide use of perturbation theory. Lemma 6 gives such an upper bound. The proof of Proposition 4 is then a direct result of Equations (19), (20), (21) and Lemma 6.

Lemma 6. *The following inequality holds*

$$\begin{aligned} \mathbb{E}\|(\widehat{\Pi}_{m_2} - \Pi_{m_2})S\Pi_{m_1}\Gamma^{1/2}\|_{\text{HS}}^2 &\leq \frac{Cm_2\lambda_{m_2}}{n} + \frac{Cm_2^2\ln(m_2)}{n\psi_\beta(m_2)} + \frac{Cm_2^3}{n\psi_\beta(\lfloor m_2/2 \rfloor)} + \frac{C\ln^2(n)}{n^2} \left(\sum_{k=1}^{m_2} \frac{k^2\ln^2(k)}{\sqrt{\psi_\beta(k)}} \right)^2 \\ &\quad + \frac{C}{n^2}\|S\Gamma^{1/2}\|_{\text{HS}}^2. \end{aligned}$$

Proof of Lemma 6. According to Lemma 2, we have

$$(\widehat{\Pi}_{m_2} - \Pi_{m_2})\mathbf{1}_{\mathcal{A}_n} = \mathcal{H}_n(z) + \mathcal{G}_n(z),$$

where the operators $\mathcal{H}_n(z)$ and $\mathcal{G}_n(z)$ are defined as

$$\begin{aligned} \mathcal{H}_n(z) &= \frac{1}{2i\pi} \sum_{k=1}^{m_2} \int_{\mathcal{B}_k} R(z)(\Gamma_n - \Gamma)R(z)dz\mathbf{1}_{\mathcal{A}_n}, \\ \mathcal{G}_n(z) &= \frac{1}{2i\pi} \sum_{k=1}^{m_2} \int_{\mathcal{B}_k} R^{1/2}(z)[I - T_n(z)]^{-1}T_n(z)^2R^{1/2}(z)dz\mathbf{1}_{\mathcal{A}_n}, \end{aligned}$$

with $T_n(z) = R^{1/2}(z)(\Gamma_n - \Gamma)R^{1/2}(z)$ and $R(z) = (zI - \Gamma)^{-1}$. Then,

$$\begin{aligned} \mathbb{E}\|(\widehat{\Pi}_{m_2} - \Pi_{m_2})S\Pi_{m_1}\Gamma^{1/2}\|_{\text{HS}}^2 &\leq 2\mathbb{E}\|\mathcal{H}_n(z)S\Pi_{m_1}\Gamma^{1/2}\|_{\text{HS}}^2 + 2\mathbb{E}\|\mathcal{G}_n(z)S\Pi_{m_1}\Gamma^{1/2}\|_{\text{HS}}^2 \\ &\quad + \mathbb{E}\|(\widehat{\Pi}_{m_2} - \Pi_{m_2})S\Pi_{m_1}\Gamma^{1/2}\mathbf{1}_{\mathcal{A}_n^c}\|_{\text{HS}}^2. \end{aligned} \quad (22)$$

Upper bounding the expectations of Equation (22) is technical and the remainder of the proof is quite long. Since $\mathcal{H}_n(z)$ is self-adjoint, we write

$$\begin{aligned} \mathbb{E}\|\mathcal{H}_n(z)S\Pi_{m_1}\Gamma^{1/2}\|_{\text{HS}}^2 &= \sum_{j=1}^{m_1} \sum_{l=1}^{+\infty} \lambda_j \mathbb{E}\langle \mathcal{H}_n(z)S(\varphi_j), \varphi_l \rangle^2 \\ &= \sum_{j=1}^{m_1} \sum_{l=1}^{+\infty} \lambda_j \mathbb{E}\langle S(\varphi_j), \mathcal{H}_n(z)(\varphi_l) \rangle^2. \end{aligned} \quad (23)$$

Furthermore, for j, l in $\mathbb{N} \setminus \{0\}$, we have

$$\begin{aligned} \langle S(\varphi_j), \mathcal{H}_n(z)(\varphi_l) \rangle &= \sum_{r=1}^{+\infty} \langle S(\varphi_j), \varphi_r \rangle \langle \mathcal{H}_n(z)(\varphi_l), \varphi_r \rangle \\ &= \sum_{r=1}^{+\infty} \langle S(\varphi_j), \varphi_r \rangle \times \frac{1}{2i\pi} \sum_{k=1}^{m_2} \int_{\mathcal{B}_k} \langle R(z)(\Gamma_n - \Gamma)R(z)(\varphi_l), \varphi_r \rangle dz\mathbf{1}_{\mathcal{A}_n}. \end{aligned}$$

Now, it is straightforward to show that $R(z)(\varphi_\ell) = (z - \lambda_\ell)^{-1}\varphi_\ell$. This together with the fact that $R(z)$ is self-adjoint, gives

$$\begin{aligned} \langle S(\varphi_j), \mathcal{H}_n(z)(\varphi_l) \rangle &= \sum_{r=1}^{+\infty} \langle S(\varphi_j), \varphi_r \rangle \langle (\Gamma_n - \Gamma)(\varphi_l), \varphi_r \rangle \times \frac{1}{2i\pi} \sum_{k=1}^{m_2} \int_{\mathcal{B}_k} (z - \lambda_l)^{-1} (z - \lambda_r)^{-1} dz \mathbf{1}_{\mathcal{A}_n} \\ &= \sum_{r=1}^{+\infty} \langle S(\varphi_j), \varphi_r \rangle \langle (\Gamma_n - \Gamma)(\varphi_l), \varphi_r \rangle \mathcal{I}_{m_2, l, r} \mathbf{1}_{\mathcal{A}_n}, \end{aligned}$$

where $\mathcal{I}_{m_2, l, r} = \frac{1}{2i\pi} \sum_{k=1}^{m_2} \int_{\mathcal{B}_k} (z - \lambda_l)^{-1} (z - \lambda_r)^{-1} dz$. The integral sum $\mathcal{I}_{m_2, l, r}$ can be computed using Cauchy's integral formula (Rudin, 1987). Indeed,

$$\begin{aligned} \mathcal{I}_{m_2, l, r} &= \frac{1}{\lambda_l - \lambda_r} \times \frac{1}{2i\pi} \sum_{k=1}^{m_2} \int_{\mathcal{B}_k} \left[\frac{1}{z - \lambda_l} - \frac{1}{z - \lambda_r} \right] dz \\ &= \frac{1}{\lambda_l - \lambda_r} \sum_{k=1}^{m_2} [\text{Ind}_{\mathcal{B}_k}(\lambda_l) - \text{Ind}_{\mathcal{B}_k}(\lambda_r)], \end{aligned}$$

where $\text{Ind}_{\mathcal{B}_k}$ is an integer-valued function, taking 1 if its argument belongs to the surface drawn by \mathcal{B}_k and 0 otherwise. Then,

$$\mathcal{I}_{m_2, l, r} = \frac{1}{\lambda_l - \lambda_r} [\mathbf{1}_{l \in \{1, \dots, m_2\}} - \mathbf{1}_{r \in \{1, \dots, m_2\}}].$$

We turn back to Equation (23). Since $\langle \Gamma \varphi_j, \varphi_r \rangle = 0$ if $j \neq r$, we can write

$$\mathbb{E} \|\mathcal{H}_n(z) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 = \mathbb{E}[A \mathbf{1}_{\mathcal{A}_n}] + \mathbb{E}[B \mathbf{1}_{\mathcal{A}_n}],$$

where A and B are defined as

$$\begin{aligned} A &= \sum_{j=1}^{m_1} \lambda_j \sum_{l=1}^{m_2} \left[\sum_{r=m_2+1}^{+\infty} \frac{\langle \Gamma_n(\varphi_l), \varphi_r \rangle}{\lambda_l - \lambda_r} \langle S(\varphi_j), \varphi_r \rangle \right]^2, \\ B &= \sum_{j=1}^{m_1} \lambda_j \sum_{l=m_2+1}^{+\infty} \left[\sum_{r=1}^{m_2} \frac{\langle \Gamma_n(\varphi_l), \varphi_r \rangle}{\lambda_r - \lambda_l} \langle S(\varphi_j), \varphi_r \rangle \right]^2. \end{aligned}$$

This implies that

$$\mathbb{E} \|\mathcal{H}_n(z) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 \leq \mathbb{E}[A] + \mathbb{E}[B]. \quad (24)$$

Thanks to Assumption \mathcal{A}_6 , while developing the sum squares in A and B , the expectation of the cross terms equals zero. In fact, for r, r' in $\mathbb{N} \setminus \{0\}$ and ℓ in $\mathbb{N} \setminus \{0, r, r'\}$, we write

$$\begin{aligned} \mathbb{E} \langle \Gamma_n(\varphi_l), \varphi_r \rangle \langle \Gamma_n(\varphi_l), \varphi_{r'} \rangle &= \frac{1}{n^2} \sum_{i=1}^n \sum_{i'=1}^n \mathbb{E} \langle X_i \otimes X_i(\varphi_l), \varphi_r \rangle \langle X_{i'} \otimes X_{i'}(\varphi_l), \varphi_{r'} \rangle \\ &= \frac{1}{n^2} \sum_{i=1}^n \mathbb{E} \langle X_i, \varphi_r \rangle \langle X_i, \varphi_{r'} \rangle \mathbb{E} \langle X_i, \varphi_l \rangle^2 \\ &= \mathbf{1}_{\{r=r'\}} \frac{\lambda_r \lambda_l}{n}. \end{aligned}$$

Therefore,

$$\mathbb{E}[A] = \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=m_2+1}^{+\infty} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S \Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \quad (25)$$

From here, we split the sum above in two parts as follows

$$\begin{aligned} \mathbb{E}[A] &= \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=m_2+1}^{2m_2} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S \Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\quad + \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=2m_2+1}^{+\infty} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S \Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned} \quad (26)$$

To upper bound the first right-side term of Equation (26), we begin with

$$\begin{aligned} & \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=m_2+1}^{2m_2} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ & \leq \frac{1}{n} \sum_{l=1}^{m_2} \sum_{u=m_2+1}^{2m_2} \frac{\lambda_l \lambda_u}{(\lambda_l - \lambda_u)^2} \times \sum_{j=1}^{m_1} \sum_{r=m_2+1}^{2m_2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned} \quad (27)$$

Now, according to Lemma 3, we obtain

$$\begin{aligned} \sum_{l=1}^{m_2} \sum_{u=m_2+1}^{2m_2} \frac{\lambda_l \lambda_u}{(\lambda_l - \lambda_u)^2} &= \sum_{l=1}^{m_2} \sum_{u=m_2+1}^{2m_2} \frac{\lambda_l^2}{(\lambda_l - \lambda_u)^2} \times \frac{\lambda_u}{\lambda_l} \\ &\leq \sum_{l=1}^{m_2} \sum_{u=m_2+1}^{2m_2} \frac{ul}{(u-l)^2} \\ &\leq \sum_{l=1}^{m_2} \sum_{u=m_2+1}^{2m_2} \frac{2m_2^2}{(u-l)^2}. \end{aligned}$$

By making in the last sum the substitution $v := u - l$, we get

$$\begin{aligned} \sum_{l=1}^{m_2} \sum_{u=m_2+1}^{2m_2} \frac{1}{(u-l)^2} &= \sum_{l=1}^{m_2} \sum_{u=1}^{m_2} \frac{1}{(m_2 + u - l)^2} = \sum_{v=1-m_2}^{m_2-1} \frac{m_2 - |v|}{(m_2 + v)^2} \leq \sum_{v=1}^{m_2} \frac{1}{v} + \sum_{w=1}^{m_2-1} \frac{m_2 - w}{(m_2 + w)^2} \\ &\leq \sum_{v=1}^{m_2} \frac{1}{v} + 1 \leq 1 + \ln(m_2). \end{aligned}$$

We turn back to Equation (27) and we write

$$\begin{aligned} \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=m_2+1}^{2m_2} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 &\leq \frac{Cm_2^2 \ln(m_2)}{n} \sum_{j=1}^{m_1} \sum_{r=m_2+1}^{2m_2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\leq \frac{Cm_2^2 \ln(m_2)}{n} \sum_{j=1}^{m_1} \sum_{r=m_2+1}^{2m_2} \frac{\psi_\beta(r)}{\psi_\beta(m_2)} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned}$$

In other words,

$$\frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=m_2+1}^{2m_2} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \leq \frac{Cm_2^2 \ln(m_2)}{n\psi_\beta(m_2)}. \quad (28)$$

We now deal with the second term of Equation (26). From Lemma 3, for $l \leq m_2$ and $r \geq 2m_2 + 1$, we have

$$\frac{\lambda_l^2}{(\lambda_l - \lambda_r)^2} \leq \frac{1}{(1 - l/r)^2} \leq \frac{1}{[1 - m_2/(2m_2 + 1)]^2} \leq 4. \quad (29)$$

Thus,

$$\begin{aligned} \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=2m_2+1}^{+\infty} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 &\leq \frac{4}{n} \sum_{l=1}^{m_2} \sum_{j=1}^{m_1} \sum_{r=2m_2+1}^{+\infty} \frac{\lambda_r}{\lambda_l} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\leq \frac{Cm_2}{n} \sum_{l=1}^{m_2} \frac{1}{\lambda_l} \sum_{u=2m_2+1}^{+\infty} \lambda_u \times \sum_{j=1}^{m_1} \sum_{r=2m_2+1}^{+\infty} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\leq \frac{Cm_2}{n} \sum_{l=1}^{m_2} \frac{\lambda_{2m_2+1}}{\lambda_l} \times \sum_{j=1}^{m_1} \sum_{r=2m_2+1}^{+\infty} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2, \end{aligned}$$

where the latter inequality is achieved thanks to Lemma 3. Subsequently,

$$\begin{aligned} \frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=2m_2+1}^{+\infty} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 &\leq \frac{Cm_2^2}{n} \sum_{j=1}^{m_1} \sum_{r=2m_2+1}^{+\infty} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\leq \frac{Cm_2^2}{n\psi_\beta(m_2)} \sum_{j=1}^{m_1} \sum_{r=2m_2+1}^{+\infty} \psi_\beta(r) \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned}$$

Simply put that

$$\frac{1}{n} \sum_{j=1}^{m_1} \sum_{l=1}^{m_2} \sum_{r=2m_2+1}^{+\infty} \frac{\lambda_l \lambda_r}{(\lambda_l - \lambda_r)^2} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \leq \frac{Cm_2^2}{n\psi_\beta(m_2)}. \quad (30)$$

As a result of Equations (26), (28) and (30), we get

$$\mathbb{E}[A] \leq \frac{Cm_2^2 \ln(m_2)}{n\psi_\beta(m_2)}. \quad (31)$$

We now upper bound the second right-side term of Equation (24). Similarly to Equation (25), we write

$$\mathbb{E}[B] = \frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=1}^{m_2} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2.$$

Next, we break the equation down into two parts as shown below

$$\begin{aligned} \mathbb{E}[B] &= \frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=1}^{\lfloor m_2/2 \rfloor} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\quad + \frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=\lfloor m_2/2 \rfloor}^{m_2} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned} \quad (32)$$

We now focus on the first right-side term of Equation (32). From the assumption $\lambda_r \psi_\beta(r) \geq 1$, we obtain

$$\begin{aligned} \frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=1}^{\lfloor m_2/2 \rfloor} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ \leq \frac{1}{n} \sum_{l=m_2+1}^{+\infty} \lambda_l \sum_{r=1}^{\lfloor m_2/2 \rfloor} \frac{\lambda_r^2}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \psi_\beta(r) \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned}$$

Similarly to Equation (29), one can show that for $l > m_2$ and $r \leq m_2/2$, we have

$$\frac{\lambda_r^2}{(\lambda_r - \lambda_l)^2} \leq C.$$

According to Lemma 3, we obtain

$$\frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=1}^{\lfloor m_2/2 \rfloor} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \leq \frac{Cm_2 \lambda_{m_2}}{n}. \quad (33)$$

We next deal with the second term of Equation (32). We start with

$$\begin{aligned} \frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=\lfloor m_2/2 \rfloor}^{m_2} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ \leq \frac{1}{n\psi_\beta(\lfloor m_2/2 \rfloor)} \sum_{l=m_2+1}^{+\infty} \lambda_l \times \sum_{r=\lfloor m_2/2 \rfloor}^{m_2} \frac{\lambda_r}{(\lambda_r - \lambda_{m_2+1})^2} \sum_{j=1}^{m_1} \psi_\beta(r) \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ \leq \frac{Cm_2}{n\psi_\beta(\lfloor m_2/2 \rfloor)} \sum_{r=\lfloor m_2/2 \rfloor}^{m_2} \frac{\lambda_r \lambda_{m_2+1}}{(\lambda_r - \lambda_{m_2+1})^2} \sum_{j=1}^{m_1} \psi_\beta(r) \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2. \end{aligned}$$

Still using Lemma 3, for $l > m_2$ and $\lfloor m_2/2 \rfloor \leq r \leq m_2$ we have that

$$\frac{\lambda_r \lambda_{m_2+1}}{(\lambda_r - \lambda_{m_2+1})^2} \leq C m_2^2.$$

Consequently,

$$\frac{1}{n} \sum_{l=m_2+1}^{+\infty} \sum_{r=\lfloor m_2/2 \rfloor}^{m_2} \frac{\lambda_r \lambda_l}{(\lambda_r - \lambda_l)^2} \sum_{j=1}^{m_1} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \leq \frac{C m_2^3}{n \psi_\beta(\lfloor m_2/2 \rfloor)}. \quad (34)$$

From Equations (33) and (34), we conclude that

$$\mathbb{E}[B] \leq \frac{C m_2 \lambda_{m_2}}{n} + \frac{C m_2^3}{n \psi_\beta(\lfloor m_2/2 \rfloor)}. \quad (35)$$

Subsequently, from Equations (24), (31) and (35), we write

$$\mathbb{E} \|\mathcal{H}_n(z) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 \leq \frac{C m_2 \lambda_{m_2}}{n} + \frac{C m_2^2 \ln(m_2)}{n \psi_\beta(m_2)} + \frac{C m_2^3}{n \psi_\beta(\lfloor m_2/2 \rfloor)}. \quad (36)$$

To upper bound the second right-side term of Equation (22), we draw inspiration from the proof of Lemma 15 of Brunel et al. (2016). We write

$$\begin{aligned} \|\mathcal{G}_n(z) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 &= \frac{1}{4\pi^2} \sum_{j=1}^{m_1} \|\mathcal{G}_n(z) S \Gamma^{1/2}(\varphi_j)\|^2 \\ &\leq \frac{1}{4\pi^2} \sum_{j=1}^{m_1} \left(\sum_{k=1}^{m_2} \int_{\mathcal{B}_k} \|R^{1/2}(z) [I - T_n(z)]^{-1} T_n(z)^2 R^{1/2}(z) S \Gamma^{1/2}(\varphi_j)\| \right)^2 \end{aligned}$$

We introduce the diagonal operator P_β defined for all j in $\mathbb{N} \setminus \{0\}$ by

$$P_\beta(\varphi_j) = \psi_\beta(j)^{1/2} \varphi_j.$$

Then,

$$\begin{aligned} &\|\mathcal{G}_n(z) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 \\ &\leq \frac{1}{4\pi^2} \sum_{j=1}^{m_1} \left(\sum_{k=1}^{m_2} \int_{\mathcal{B}_k} \|R^{1/2}(z)\|_\infty \| [I - T_n(z)]^{-1} \|_\infty \|T_n(z)\|_\infty^2 \|R^{1/2}(z) P_\beta^{-1}\|_\infty \|P_\beta S \Gamma^{1/2}(\varphi_j)\| \right)^2 \end{aligned}$$

From here we use some results of Brunel et al. (2016), page 226. In particular, on the set \mathcal{A}_n and for z in \mathcal{B}_k , we write

$$\| [I - T_n(z)]^{-1} \|_\infty < 2 \quad \text{and} \quad \|T_n(z)\|_\infty \leq \frac{\mathbf{a}_k}{\sqrt{n}} \ln(n).$$

Also, remark that for z in \mathcal{B}_k , we have

$$\begin{aligned} \|R^{1/2}(z) P_\beta^{-1}\|_\infty &= \sup_{l \in \mathbb{N} \setminus \{0\}} \psi_\beta(l)^{-1/2} |z - \lambda_l|^{-1/2} \\ &= \psi_\beta(k)^{-1/2} \sqrt{2/\delta_k}. \end{aligned}$$

Hence,

$$\begin{aligned} \|\mathcal{G}_n(z) S \Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 &\leq \frac{C \ln^4(n)}{n^2} \sum_{j=1}^{m_1} \|P_\beta S \Gamma^{1/2}(\varphi_j)\|^2 \left(\sum_{k=1}^{m_2} \mathbf{a}_k^2 \psi_\beta(k)^{-1/2} \right)^2 \\ &= \frac{C \ln^4(n)}{n^2} \|P_\beta S \Gamma^{1/2}\|_{\text{HS}}^2 \left(\sum_{k=1}^{m_2} \mathbf{a}_k^2 \psi_\beta(k)^{-1/2} \right)^2. \end{aligned}$$

Besides, according to Lemma 4, under Assumptions \mathcal{A}_2 and \mathcal{A}_6 , we have $\mathbf{a}_k \leq Ck \ln(k)$. Furthermore,

$$\|P_\beta S\Gamma^{1/2}\|_{\text{HS}}^2 = \sum_{j=1}^{+\infty} \sum_{l=1}^{+\infty} \psi_\beta(l) \langle S\Gamma^{1/2}(\varphi_j), \varphi_l \rangle^2 < +\infty.$$

Therefore,

$$\mathbb{E} \|\mathcal{G}_n(z) S\Pi_{m_1} \Gamma^{1/2}\|_{\text{HS}}^2 \leq \frac{C \ln^4(n)}{n^2} \left(\sum_{k=1}^{m_2} \frac{k^2 \ln^2(k)}{\sqrt{\psi_\beta(k)}} \right)^2. \quad (37)$$

To end this proof, we provide an upper bound for the remaining term of Equation (22). It is plain that

$$\mathbb{E} \|(\widehat{\Pi}_{m_2} - \Pi_{m_2}) S\Pi_{m_1} \Gamma^{1/2} \mathbf{1}_{\mathcal{A}_n^c}\|_{\text{HS}}^2 \leq 4 \|S\Gamma^{1/2}\|_{\text{HS}}^2 \mathbb{P}(\mathbf{1}_{\mathcal{A}_n^c}).$$

It follows from Lemma 2 that

$$\mathbb{E} \|(\widehat{\Pi}_{m_2} - \Pi_{m_2}) S\Pi_{m_1} \Gamma^{1/2} \mathbf{1}_{\mathcal{A}_n^c}\|_{\text{HS}}^2 \leq \frac{C}{n^2} \|S\Gamma^{1/2}\|_{\text{HS}}^2. \quad (38)$$

At last, combining Equations (22), (36), (37) and (38) leads to the required result.

6.3.2 Proof of Corollary 1

From Equation (10), the minimax prediction rate is lower than the infimum of the right-side term with respect to m_1 and m_2 . Let us consider the terms of the upper-bound successively.

- We keep the first one, $\sigma_\varepsilon^2 m_1/n$.
- For the second term, under Assumption \mathcal{A}_1 , we obtain

$$\begin{aligned} \sum_{j=m_1+1}^{+\infty} \|S\Gamma^{1/2}(\varphi_j)\|^2 &= \sum_{j=m_1+1}^{+\infty} \sum_{r=1}^{+\infty} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\leq \sum_{j=m_1+1}^{+\infty} \sum_{r=1}^{+\infty} \frac{\eta_\alpha(j)}{\eta_\alpha(m_1)} \langle S\Gamma^{1/2}(\varphi_j), \varphi_r \rangle^2 \\ &\leq c/\eta_\alpha(m_1), \end{aligned}$$

where c is some positive constant.

- The third term, $\sum_{j=1}^{m_1} \|(I - \Pi_{m_2}) S\Gamma^{1/2}(\varphi_j)\|^2$ goes to zero when m_2 goes to $+\infty$.
- We have $A_{n,m_1} \leq \sigma_\varepsilon^2 m_1/n$ under the constraint $m_1 \leq n/\ln^2(n)$.
- The additional assumption $\lambda_{m_1} \leq m_1^{-1-\nu}$ permits to obtain that B_{n,m_1} is negligible with respect to $\sigma_\varepsilon^2 m_1/n$.
- The term E_n is immediately negligible with respect to $1/n$.
- From the convergence of $\sum_{m_2 \geq 1} \lambda_{m_2}$, the first term of D_{n,m_2} goes to 0 when m_2 goes to $+\infty$. The same result applies to the second and third terms of D_{n,m_2} in view of the assumptions on ψ_β .
- The last term of D_{n,m_2} is lower to $c \ln^4(n)/n^2$ (and thus to c/n). Indeed, from the assumptions on ψ_β , the serie $\sum_{k \geq 1} k^2 \ln^2(k)/\sqrt{\psi_\beta(k)}$ is convergent.

6.3.3 Proof of Theorem 2

To lower bound the minimax risk, we follow the general scheme of reduction to a finite hypotheses number, as described in [Tsybakov \(2008\)](#). Our approach is similar to the one applied in [Crambes and Mas \(2013\)](#), but the regularity assumption differs, making it necessary to adapt the proof significantly. We start by considering a family of hypothesis S^θ of S , indexed by θ in $\Omega_{m_1^*} = \{0, 1\}^{m_1^*}$. More precisely, for all $\theta = (\omega_1, \dots, \omega_{m_1^*})$ in $\Omega_{m_1^*}$, we define

$$S^\theta = \sum_{j=1}^{m_1^*} \mu_j \omega_j \varphi_1 \otimes \varphi_j,$$

where $(\mu_j)_{1 \leq j \leq m_1^*}$ are chosen in such a way that $S^\theta \Gamma^{1/2}$ belongs to $\mathcal{W}_{\alpha, \beta}^R$. Elementary computations show that we can set for all j in $\Omega_{m_1^*}$,

$$\mu_j^2 = R^2/e \times [\lambda_j m_1^* \eta_\alpha(m_1^*)]^{-1}.$$

Besides, it is straightforward to see that

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha, \beta}^R} \mathbb{E} \|\widehat{S}_n(X_{n+1}) - S(X_{n+1})\|^2 \geq \inf_{\widehat{S}_n} \max_{\theta \in \Omega_{m_1^*}} \mathbb{E} \|\widehat{S}_n(X_{n+1}) - S^\theta(X_{n+1})\|^2. \quad (39)$$

For a given estimator \widehat{S}_n , let $\widehat{\theta}(\widehat{S}_n)$ be a random vector verifying that

$$\widehat{\theta}(\widehat{S}_n) \in \arg \min_{\theta \in \Omega_{m_1^*}} \mathbb{E} \|\widehat{S}_n(X_{n+1}) - S^\theta(X_{n+1})\|^2.$$

The model $S^{\widehat{\theta}(\widehat{S}_n)}$ is one of the nearest to \widehat{S}_n , among the collection $\{S^\theta; \theta \in \Omega_{m_1^*}\}$. Then, for all θ in $\Omega_{m_1^*}$,

$$\begin{aligned} \mathbb{E} \|S^{\widehat{\theta}(\widehat{S}_n)}(X_{n+1}) - S^\theta(X_{n+1})\|^2 &\leq 2\mathbb{E} \|\widehat{S}_n(X_{n+1}) - S^{\widehat{\theta}(\widehat{S}_n)}(X_{n+1})\|^2 + 2\mathbb{E} \|\widehat{S}_n(X_{n+1}) - S^\theta(X_{n+1})\|^2 \\ &\leq 4\mathbb{E} \|\widehat{S}_n(X_{n+1}) - S^\theta(X_{n+1})\|^2. \end{aligned}$$

Therefore, using Equation (39), we get

$$\begin{aligned} \inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha, \beta}^R} \mathbb{E} \|\widehat{S}_n(X_{n+1}) - S(X_{n+1})\|^2 &\geq \frac{1}{4} \inf_{\widehat{S}_n} \max_{\theta \in \Omega_{m_1^*}} \mathbb{E} \|S^{\widehat{\theta}(\widehat{S}_n)}(X_{n+1}) - S^\theta(X_{n+1})\|^2 \\ &\geq \frac{1}{4} \inf_{\widehat{\theta}} \max_{\theta \in \Omega_{m_1^*}} \mathbb{E} \|S^{\widehat{\theta}}(X_{n+1}) - S^\theta(X_{n+1})\|^2, \end{aligned} \quad (40)$$

where the infimum in the last line is taken over the all the estimators with values in $\Omega_{m_1^*}$. From here, we aim to apply Assouad's Lemma with Kullback version, see [Tsybakov \(2008, pages 117 to 119\)](#). For the sake of completeness, we recall below this lemma.

Lemma 7 (Assouad version Kullback-Leibler). *Let ρ denotes the Hamming distance, defined for all $\theta = (\omega_1, \dots, \omega_m)$ and $\theta' = (\omega'_1, \dots, \omega'_m)$ in $\Omega_m = \{0, 1\}^m$ by*

$$\rho(\theta, \theta') = \sum_{j=1}^m \mathbb{1}_{\{\omega_j \neq \omega'_j\}}.$$

We also denote by $\mathbb{P}_\theta^{\otimes n}$ the distribution of $(X_i, Y_i)_{1 \leq i \leq n}$ under S^θ . Assume that for all θ, θ' such that $\rho(\theta, \theta') = 1$, we have the following upper bound of the Kullback-Leibler divergence between $\mathbb{P}_\theta^{\otimes n}$ and $\mathbb{P}_{\theta'}^{\otimes n}$, $\mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n}) \leq \alpha < \infty$. Then,

$$\inf_{\widehat{\theta}} \max_{\theta \in \Omega_m} \mathbb{E}[\rho(\theta, \widehat{\theta})] \geq \frac{m}{2} \max \left(\frac{1}{2} \exp(-\alpha), 1 - \sqrt{\alpha/2} \right),$$

where the infimum is taken over all the estimators $\widehat{\theta}$ with values in Ω_m .

Now, for all estimator $\widehat{\theta} = (\widehat{\omega}_1, \dots, \widehat{\omega}_{m_1^*})$ and $\theta = (\omega_1, \dots, \omega_{m_1^*})$ both with values in $\Omega_{m_1^*}$, we write

$$\begin{aligned} \mathbb{E}\|S^{\widehat{\theta}}(X_{n+1}) - S^\theta(X_{n+1})\|^2 &= \mathbb{E}\left\|\sum_{j=1}^{m_1^*} \mu_j(\widehat{\omega}_j - \omega_j)\varphi_1 \otimes \varphi_j(X_{n+1})\right\|^2 \\ &= \mathbb{E}\left\|\sum_{j=1}^{m_1^*} \mu_j(\widehat{\omega}_j - \omega_j)\varphi_1 \otimes \varphi_j\Gamma^{1/2}\right\|_{\text{HS}}^2, \end{aligned}$$

where the last equation stems from Lemma 5. Thus,

$$\begin{aligned} \mathbb{E}\|S^{\widehat{\theta}}(X_{n+1}) - S^\theta(X_{n+1})\|^2 &= \sum_{j=1}^{m_1^*} \lambda_j \mu_j^2 \mathbb{E}[(\widehat{\omega}_j - \omega_j)^2] \\ &= R^2/e \times [m_1^* \eta_\alpha(m_1^*)]^{-1} \mathbb{E}[\rho(\theta, \widehat{\theta})]. \end{aligned}$$

We then get from Equation (40) that

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha, \beta}^R} \mathbb{E}\|\widehat{S}_n(X_{n+1}) - S(X_{n+1})\|^2 \geq \frac{R^2}{4e} [m_1^* \eta_\alpha(m_1^*)]^{-1} \inf_{\widehat{\theta}} \max_{\theta \in \Omega_{m_1^*}} \mathbb{E}[\rho(\theta, \widehat{\theta})]. \quad (41)$$

In order to apply Assouad's Lemma, we now upper bound $\mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n})$ for θ, θ' such that $\rho(\theta, \theta') = 1$. We are aware that the definition of the last Kullback-Leibler divergence requires that $\mathbb{P}_\theta^{\otimes n}$ is absolutely continuous with respect to $\mathbb{P}_{\theta'}^{\otimes n}$. This point will be clarified later. Furthermore, it is well known that

$$\mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n}) = n \mathbf{KL}(\mathbb{P}_\theta, \mathbb{P}_{\theta'}),$$

where \mathbb{P}_θ is the distribution of (X, Y^θ) , with $Y^\theta = S^\theta X + \varepsilon$. Then,

$$\begin{aligned} \mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n}) &= n \int \ln \left(\frac{d\mathbb{P}_\theta}{d\mathbb{P}_{\theta'}} \right) d\mathbb{P}_\theta \\ &= n \int \left[\int \ln \left(\frac{d\mathbb{P}_{Y^\theta|X}}{d\mathbb{P}_{Y^{\theta'}|X}} \right) d\mathbb{P}_{Y^\theta|X} \right] d\mathbb{P}_X. \end{aligned}$$

The absolute continuity of $\mathbb{P}_{Y^\theta|X}$ with respect to $\mathbb{P}_{Y^{\theta'}|X}$ and the upper bound of the Kullback-Leibler divergence are provided by Cameron–Martin Theorem (Lifshits, 2012), which is stated below.

Theorem 4 (Cameron–Martin). *Let Z be a centered Gaussian random variable in a Hilbert space $(\mathcal{X}, \langle \cdot, \cdot \rangle, \|\cdot\|)$, with a distribution measure P and a covariance operator Γ_Z . We consider the subset $H_P \subset \mathcal{X}$ defined as*

$$H_P = \left\{ h \in \mathcal{X} \text{ such that } \|\Gamma_Z^{-1/2}(h)\|^2 < +\infty \right\}.$$

For all h in H_P , we denote by P_h the distribution measure of $Z + h$. Then, P_h is absolutely continuous with respect to P and the density dP_h/dP is given by

$$dP_h/dP : x \mapsto \exp \left\{ \langle x, \Gamma_Z^{-1}(h) \rangle - \frac{1}{2} \|\Gamma_Z^{-1/2}(h)\|^2 \right\}.$$

The next step is to apply Cameron-Martin Theorem to upper bound $\mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n})$. Before this, there are some points to specify. We denote for the remaining of the proof Γ_ε , the covariance operator of ε . It is quite easy to see that conditionally to X , the distribution of Y_θ is Gaussian with mean $S^\theta X$ and covariance operator $\Gamma_{Y_\theta} = \Gamma_\varepsilon$. Let us set $h_\theta = S^\theta X$, for all θ in $\Omega_{m_1^*}$. Then, conditionally to X , the random variable Y^θ is a shift of $Y^{\theta'}$ with a shift equal to $h^\theta - h^{\theta'}$. Therefore, according to Cameron-Martin Theorem, we have

$$\begin{aligned} \mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n}) &= n \mathbb{E}_X \mathbb{E}_\varepsilon \langle Y^\theta, \Gamma_\varepsilon^{-1}(h^\theta - h^{\theta'}) \rangle - \frac{n}{2} \mathbb{E}_X \|\Gamma_\varepsilon^{-1/2}(h^\theta - h^{\theta'})\|^2 \\ &= n \mathbb{E}_X \langle h^\theta, \Gamma_\varepsilon^{-1}(h^\theta - h^{\theta'}) \rangle - \frac{n}{2} \mathbb{E}_X \|\Gamma_\varepsilon^{-1/2}(h^\theta - h^{\theta'})\|^2, \end{aligned}$$

where \mathbb{E}_X and \mathbb{E}_ε respectively designate the expectations with respect to the distributions of X and ε . Then, according to Lemma 5, we get

$$\mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n}) = n \langle S^\theta \Gamma^{1/2}, \Gamma_\varepsilon^{-1} (S^\theta - S^{\theta'}) \Gamma^{1/2} \rangle_{\text{HS}} - \frac{n}{2} \|\Gamma_\varepsilon^{-1/2} (S^\theta - S^{\theta'}) \Gamma^{1/2}\|_{\text{HS}}^2.$$

Now, from $\rho(\theta, \theta') = 1$, we know that there exists j in $\{1, \dots, m_1^*\}$ such that $\omega_j \neq \omega'_j$ and for all $l \neq j$, $\omega_l = \omega'_l$. Thus,

$$\begin{aligned} \mathbf{KL}(\mathbb{P}_\theta^{\otimes n}, \mathbb{P}_{\theta'}^{\otimes n}) &= n \lambda_j \mu_j^2 \omega_j (\omega_j - \omega'_j) \langle \varphi_1, \Gamma_\varepsilon^{-1}(\varphi_1) \rangle - \frac{n}{2} \lambda_j \mu_j^2 \omega_j^2 \|\Gamma_\varepsilon^{-1/2}(\varphi_1)\|^2 \\ &= \frac{R^2}{2e\sigma_1} \omega_j (\omega_j - 2\omega'_j) \times \frac{n}{m_1^* \eta_\alpha(m_1^*)} \\ &\leq \frac{R^2}{2e\sigma_1} \times \frac{n}{m_1^* \eta_\alpha(m_1^*)}, \end{aligned}$$

where $1/\sigma_1 = \|\Gamma_\varepsilon^{-1/2}(\varphi_1)\|^2$. Bearing in mind that $m_1^* \eta_\alpha(m_1^*) \geq n/c_0$, for some positive constant c_0 . By fitting c_0 value with respect to R , σ_1 and α , we set the condition $R^2/(2e\sigma_1) \times 1/c_0(R, \sigma_1, \alpha) \leq 1/2$. Consequently, from Assouad's Lemma and Equation (41), we get

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha, \beta}^R} \mathbb{E} \|\widehat{S}_n(X_{n+1}) - S(X_{n+1})\|^2 \geq \frac{C(R, \sigma_1, \alpha)}{\eta_\alpha(m_1^*)},$$

where $C(R, \sigma_1, \alpha)$ is some positive constant only depending on its arguments. In other words,

$$\inf_{\widehat{S}_n} \sup_{S \Gamma^{1/2} \in \mathcal{W}_{\alpha, \beta}^R} \mathbb{E} \|\widehat{S}_n(X_{n+1}) - S(X_{n+1})\|^2 \geq C(R, \sigma_1, \alpha) \inf_{m_1 \in \mathbb{N} \setminus \{0\}} \left\{ \sigma_\varepsilon^2 \frac{m_1}{n} + \frac{3}{\eta_\alpha(m_1)} \right\}.$$

6.3.4 Proof of Corollary 2

In both cases (polynomial and exponential) we have to compute $\inf_{m_1 \in \mathbb{N} \setminus \{0\}} \{\sigma_\varepsilon^2 m_1/n + 3/\eta_\alpha(m_1)\}$. We distinguish the two cases.

1. If $\eta_\alpha(x) \asymp x^\alpha$, the dimension m_1 minimizing the minimax risk is up to a multiplicative constant, the solution $x_n^* = \arg \min_{x \geq 1} R_\alpha(x)$ with $R_\alpha(x) = x/n + x^{-\alpha}$. we easily derive the result, $x_n^* = cn^{1/\alpha+1}$, for a constant c which only depends on α , and $R_\alpha(x_n^*) = cn^{-\alpha/(\alpha+1)}$, for another constant c .
2. If $\eta_\alpha(x) \asymp \exp(x^\alpha)$, we reason in a similar way with $R_\alpha(x) = x/n + \exp(-x^\alpha)$. The solution x_n^* of the minimization problem of R_α verifies the equation $\alpha(x_n^*)^{\alpha-1} e^{-(x_n^*)^\alpha} = n^{-1}$ which cannot be written explicitly except in the case $\alpha = 1$ where $x_n^* = \ln(n)$ leading to a minimax rate of order $\ln(n)/n$. In the case $\alpha \neq 1$, we can upper-bound the risk as follows, for $n \geq e^1$

$$R_\alpha(x_n^*) = \frac{x_n^*}{n} + e^{-(x_n^*)^\alpha} \leq R_\alpha\left((\ln(n))^{1/\alpha}\right) = \frac{\ln(n)^{1/\alpha}}{n} + \frac{1}{n} \leq 2 \frac{(\ln(n))^{1/\alpha}}{n}$$

implying that there exists $c > 0$ such that, for n large enough, $e^{-(x_n^*)^\alpha} \leq 2(\ln(n))^{1/\alpha}/n$, which implies

$$\begin{aligned} x_n^* &\geq (\ln(n) - \ln((\ln(n))^{1/\alpha} - \ln(2)))_+^{1/\alpha}, \\ &= (\ln(n))^{1/\alpha} \left(1 - \frac{1}{\alpha} \frac{\ln(\ln(n))}{n} - \frac{\ln(2)}{\ln(n)} \right)^{1/\alpha}, \\ &\geq c(\ln(n))^{1/\alpha}. \end{aligned}$$

Moreover,

$$R_\alpha(x_n^*) = \frac{x_n^*}{n} + e^{-(x_n^*)^\alpha} \geq \frac{x_n^*}{n} \geq c \frac{(\ln(n))^{1/\alpha}}{n}.$$

Then the minimax rate is larger than $(\ln(n))^{1/\alpha}/n$.

6.4 Proof of the results of Section 4

6.4.1 Proof of Theorem 3

Starting from the definition of \widehat{m}_1 , we have for all m_1 in \mathcal{M}_n that

$$\gamma_n(\widehat{S}_{\widehat{m}_1, \infty}) \leq \gamma_n(\widehat{S}_{m_1, \infty}) + \text{pen}(m_1) - \text{pen}(\widehat{m}_1). \quad (42)$$

Moreover, $\widehat{S}_{m_1, \infty}$ is the limit, in the sense of the Hilbert-Schmidt norm of \widehat{S}_{m_1, m_2} when m_2 goes to infinity. Since the contrast function $\gamma_n : \mathcal{L}_2(\mathbb{H}) \rightarrow \mathbb{R}$ is continuous (where we recall that $\mathcal{L}_2(\mathbb{H})$ is the space of Hilbert-Schmidt operators of $\mathbb{H} = L^2([0, 1])$), then

$$\gamma_n(\widehat{S}_{m_1, \infty}) = \lim_{m_2 \rightarrow \infty} \gamma_n(\widehat{S}_{m_1, m_2}) \leq \lim_{m_2 \rightarrow \infty} \gamma_n(\widehat{\Pi}_{m_1, m_2} S) = \gamma_n(\widehat{\Pi}_{m_1, \infty} S),$$

where the inequality is a consequence of the definition of the estimators $(\widehat{S}_{m_1, m_2})_{m_1, m_2}$, see (5), and where $\widehat{\Pi}_{m_1, m_2}$ (resp. $\widehat{\Pi}_{m_1, \infty}$) stands for the projection operator onto the space $\text{Span}\{\widehat{\varphi}_k \otimes \widehat{\varphi}_j, j = 1, \dots, m_1, k = 1, \dots, m_2\}$ (resp. onto $\text{Span}\{\widehat{\varphi}_k \otimes \widehat{\varphi}_j, j = 1, \dots, m_1, k \in \mathbb{N} \setminus \{0\}\}$). Thus, since $\widehat{\Pi}_{m_1, \infty} S = S\widehat{\Pi}_{m_1}$ (where we recall that $\widehat{\Pi}_{m_1}$ is the projection operator of functions onto $\text{Span}\{\widehat{\varphi}_j, j = 1, \dots, m_1\}$, see (7)), Inequality (42) becomes

$$\gamma_n(\widehat{S}_{\widehat{m}_1, \infty}) \leq \gamma_n(S\widehat{\Pi}_{m_1}) + \text{pen}(m_1) - \text{pen}(\widehat{m}_1). \quad (43)$$

We now seek for the link between the contrast function and the empirical norm. Let T_1 and T_2 be two linear operators. Then,

$$\begin{aligned} \gamma_n(T_1) - \gamma_n(T_2) &= \frac{1}{n} \sum_{i=1}^n \|Y_i - T_1(X_i)\|^2 - \frac{1}{n} \sum_{i=1}^n \|Y_i - T_2(X_i)\|^2 \\ &= \frac{1}{n} \sum_{i=1}^n \|[S - T_1](X_i) + \varepsilon_i\|^2 - \frac{1}{n} \sum_{i=1}^n \|[S - T_2](X_i) + \varepsilon_i\|^2 \\ &= \|S - T_1\|_n^2 - \|S - T_2\|_n^2 + 2\nu_n(T_2 - T_1), \end{aligned}$$

where the empirical process ν_n is defined for any linear operator T by $\nu_n(T) = n^{-1} \sum_{i=1}^n \langle T(X_i), \varepsilon_i \rangle$. Back to Equation (42), for all m_1 in \mathcal{M}_n we write

$$\begin{aligned} \|S - \widehat{S}_{\widehat{m}_1, \infty}\|_n^2 &\leq \|S - S\widehat{\Pi}_{m_1}\|_n^2 + 2\nu_n(\widehat{S}_{\widehat{m}_1, \infty} - S\widehat{\Pi}_{m_1}) + \text{pen}(m_1) - \text{pen}(\widehat{m}_1) \\ &\leq \|S - S\widehat{\Pi}_{m_1}\|_n^2 + 2\|\widehat{S}_{\widehat{m}_1, \infty} - S\widehat{\Pi}_{m_1}\|_n \sup_{\substack{T \in V_{m_1 \vee \widehat{m}_1, \infty} \\ \|T\|_n = 1}} \nu_n(T) + \text{pen}(m_1) - \text{pen}(\widehat{m}_1), \end{aligned}$$

where for all m in $\mathbb{N} \setminus \{0\}$, $V_{m, \infty} = \text{Span}\{\widehat{\varphi}_k \otimes \widehat{\varphi}_j, j = 1, \dots, m \text{ and } k \in \mathbb{N} \setminus \{0\}\}$. Let, $\zeta > 0$ and $\tilde{\zeta} = 4\zeta^{-1} + 2$. Since $\tilde{\zeta} > 0$, we remark that for all x, y in \mathbb{R} , $2xy \leq \tilde{\zeta}x^2 + \zeta^{-1}y^2$. Then,

$$\|S - \widehat{S}_{\widehat{m}_1, \infty}\|_n^2 \leq \|S - S\widehat{\Pi}_{m_1}\|_n^2 + \tilde{\zeta}^{-1} \|\widehat{S}_{\widehat{m}_1, \infty} - S\widehat{\Pi}_{m_1}\|_n^2 + \tilde{\zeta} \sup_{\substack{T \in V_{m_1 \vee \widehat{m}_1, \infty} \\ \|T\|_n = 1}} \nu_n(T)^2 + \text{pen}(m_1) - \text{pen}(\widehat{m}_1).$$

We define for all m, m' in \mathcal{M}_n , $p(m, m') = 8\tilde{\zeta}^{-1}(1 + \delta)\sigma_\varepsilon^2(m \vee m')/n$ such that $\text{pen}(m) + \text{pen}(m') \geq \tilde{\zeta}p(m, m')$. Therefore,

$$\|S - \widehat{S}_{\widehat{m}_1, \infty}\|_n^2 \leq \|S - S\widehat{\Pi}_{m_1}\|_n^2 + \tilde{\zeta}^{-1} \|\widehat{S}_{\widehat{m}_1, \infty} - S\widehat{\Pi}_{m_1}\|_n^2 + 2\text{pen}(m_1) + \tilde{\zeta} \left(\sup_{\substack{T \in V_{m_1 \vee \widehat{m}_1, \infty} \\ \|T\|_n = 1}} \nu_n(T)^2 - p(m_1, \widehat{m}_1) \right)_+,$$

where $(\cdot)_+$ is the positive part, defined for all x in \mathbb{R} as $x_+ = x \vee 0$. Next, since

$$\|\widehat{S}_{\widehat{m}_1, \infty} - S\widehat{\Pi}_{m_1}\|_n^2 \leq 2\|\widehat{S}_{\widehat{m}_1, \infty} - S\|_n^2 + 2\|S - S\widehat{\Pi}_{m_1}\|_n^2$$

and $\tilde{\zeta} > 2$

$$(1 - 2\tilde{\zeta}^{-1})\|S - \widehat{S}_{m_1, \infty}\|_n^2 \leq (1 + 2\tilde{\zeta}^{-1})\|S - S\widehat{\Pi}_{m_1}\|_n^2 + 2\text{pen}(m_1) + \tilde{\zeta} \left(\sup_{\substack{T \in V_{m_1 \vee \widehat{m}_1, \infty} \\ \|T\|_n = 1}} \nu_n(T)^2 - p(m_1, \widehat{m}_1) \right). \quad (44)$$

The upper-bound of the expectation of the last right-sided term in Equation (44) stems from Lemma 8. This upper-bound does not depend on the selected dimension m in \mathcal{M}_n . Hence, denoting $c(\zeta) = 2(1 + 2\tilde{\zeta}^{-1})^{-1} = (2 + \zeta)/(1 + \zeta)$ we have,

$$\mathbb{E}\|S - \widehat{S}_{m_1, \infty}\|_n^2 \leq \frac{1 + 2\tilde{\zeta}^{-1}}{1 - 2\tilde{\zeta}^{-1}} \inf_{m_1 \in \mathcal{M}_n} \left\{ \mathbb{E}\|S - S\widehat{\Pi}_{m_1}\|_n^2 + c(\zeta)\text{pen}(m_1) \right\} + \frac{C(\delta, p)}{n}$$

and the result comes from the fact that $\frac{1+2\tilde{\zeta}^{-1}}{1-2\tilde{\zeta}^{-1}} = 1 + \zeta$.

Lemma 8. *Under Assumption \mathcal{A}_7 , the following inequality holds for all m in \mathcal{M}_n ,*

$$\sum_{m' \in \mathcal{M}_n} \mathbb{E} \left[\left(\sup_{\substack{T \in V_{m \vee m', \infty} \\ \|T\|_n = 1}} \nu_n^2(T) - p(m, m') \right)_+ \right] \leq \frac{C(\delta, p)}{n},$$

where $p(m, m') = 2(1 + \delta) \frac{m \vee m'}{n} \sigma^2$ and for all x in \mathbb{R} , $x_+ = x \vee 0$.

Proof of Lemma 8. The main ideas of this proof are inspired from Brunel et al. (2016, Lemma 5), with an extension of the demonstrated results in the infinite dimensional frame of this paper. Denote by $\bar{T}_X = (T(X_1), \dots, T(X_n)) \in \mathbb{H}^n$ and $\bar{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_n) \in \mathbb{H}^n$. Then,

$$\nu_n(T) = \frac{1}{n} \langle \bar{T}_X, \bar{\varepsilon} \rangle^{\otimes n},$$

where $\langle \cdot, \cdot \rangle^{\otimes n}$ is the scalar product on \mathbb{H}^n induced by $\langle \cdot, \cdot \rangle$, which is defined for all $x = (x_1, \dots, x_n)$ and $y = (y_1, \dots, y_n)$ in \mathbb{H}^n as $\langle x, y \rangle^{\otimes n} = \sum_{i=1}^n \langle x_i, y_i \rangle$. The associated norm is denoted $\|\cdot\|^{\otimes n}$. Subsequently,

$$\sup_{\substack{T \in V_{m, \infty} \\ \|T\|_n = 1}} \nu_n(T) = \sup_{\substack{z \in \widetilde{V}_{m, \infty} \\ \|z\|^{\otimes n} = \sqrt{n}}} \frac{1}{n} \langle z, \bar{\varepsilon} \rangle^{\otimes n},$$

where $\widetilde{V}_{m, \infty}$ is the linear subspace of \mathbb{H}^n defined as

$$\widetilde{V}_{m, \infty} = \{z \in \mathbb{H}^n, \exists T \in V_{m, \infty} \text{ such that } z = \bar{T}_X\}.$$

Therefore, denoting by $\Pi_{\widetilde{V}_{m, \infty}}^{\otimes n}$ the orthogonal projection onto $\widetilde{V}_{m, \infty}$, we get

$$\sup_{\substack{T \in V_{m, \infty} \\ \|T\|_n = 1}} \nu_n(T) = \frac{1}{\sqrt{n}} \sup_{\substack{z \in \widetilde{V}_{m, \infty} \\ \|z\|^{\otimes n} = 1}} \langle z, \bar{\varepsilon} \rangle^{\otimes n} = \frac{1}{\sqrt{n}} \|\Pi_{\widetilde{V}_{m, \infty}}^{\otimes n}(\bar{\varepsilon})\|^{\otimes n}.$$

From here, we use the Talagrand-type inequality stated in Lemma 9, which is an adaptation of (Baraud, 2000, Corollary 5.1) in our setting. For all $x > 0$, we write

$$\mathbb{P} \left(n \sup_{\substack{T \in V_{m, \infty} \\ \|T\|_n = 1}} \nu_n^2(T) \geq m\sigma_\varepsilon^2 + 2\sigma_\varepsilon^2 \sqrt{mx} + \sigma_\varepsilon^2 x \right) \leq C(p) \sigma_\varepsilon^p \tau_p \frac{m}{x^{p/2}},$$

where $\tau_p = \mathbb{E}\|\varepsilon\|^p$. Now, for all $\theta > 0$, notice that $2\sqrt{mx} \leq \theta m + \theta^{-1}x$, this means that

$$\mathbb{P}\left(\sup_{\substack{T \in V_{m,\infty} \\ \|T\|_n=1}} \nu_n^2(T) \geq (1+\theta)\frac{m\sigma_\varepsilon^2}{n} + (1+\theta^{-1})\frac{\sigma_\varepsilon^2 x}{n}\right) \leq C(p)\frac{m}{x^{p/2}},$$

We set,

$$Q_{m \vee m'} = \left(\sup_{\substack{T \in V_{m \vee m', \infty} \\ \|T\|_n=1}} \nu_n^2(T) - p(m, m') \right)_+.$$

We write for all m, m' in \mathcal{M}_n ,

$$\begin{aligned} \mathbb{E}[Q_{m \vee m'}] &= \int_0^{+\infty} \mathbb{P}(Q_{m \vee m'} \geq t) dt \\ &\leq C(\delta, p) \frac{m \vee m'}{n^{p/2}} \int_0^{+\infty} \frac{dt}{(t + \sigma_\varepsilon^2 m \vee m' / n(1 + \delta))^{p/2}} \leq C(\delta, p)(m \vee m')^{2-p/2}/n. \end{aligned}$$

Knowing that $p > 4$, we have that $(m \vee m')^{2-p/2} \leq 1$ which gives the desired result.

Lemma 9. *Let L be a linear subspace of \mathbb{H}^n and $m \in \mathbb{N} \setminus \{0\}$ such that $\dim(L) \leq m$. Denote by ζ the map defined on \mathbb{H}^n as*

$$\zeta : s \mapsto \|\Pi_L^{\otimes n}(s)\|^{\otimes n},$$

where $\Pi_L^{\otimes n}$ designates the orthogonal projection onto L with respect to $\langle \cdot, \cdot \rangle^{\otimes n}$. Then, for all $p \geq 2$ such that $\tau_p = \mathbb{E}\|\varepsilon\|^p < +\infty$ and for all $x > 0$, we have

$$\mathbb{P}(\zeta^2(\bar{\varepsilon}) \geq m\sigma_\varepsilon^2 + 2\sigma_\varepsilon^2\sqrt{mx} + \sigma_\varepsilon^2 x) \leq C(p)\frac{m}{x^{p/2}}.$$

Proof of Lemma 9. Let (ψ_1, \dots, ψ_m) be an orthonormal basis of L , with $m \leq n$. Denote by \mathcal{B}_n the unit ball of \mathbb{H}^n with respect to the norm $\|\cdot\|^{\otimes n}$, we have

$$\begin{aligned} \zeta^2(\bar{\varepsilon}) &= \left[\sup_{u \in \mathcal{B}_n} \langle \Pi_L^{\otimes n}(\bar{\varepsilon}), u \rangle^{\otimes n} \right]^2 = \left[\sup_{u \in \mathcal{B}_n} \langle \bar{\varepsilon}, \Pi_L^{\otimes n}(u) \rangle^{\otimes n} \right]^2 \\ &= \left[\sup_{u \in \mathcal{B}_n} \sum_{j=1}^m \langle \bar{\varepsilon}, \psi_j \rangle^{\otimes n} \langle u, \psi_j \rangle^{\otimes n} \right]^2. \end{aligned}$$

Let v_i be the n -tuple of \mathbb{H}^n composed by ε_i in the i^{th} position and $0_{\mathbb{H}}$ elsewhere. By construction, $(v_i)_i$ are independent and $\bar{\varepsilon} = \sum_{i=1}^n v_i$ and if we denote for u in \mathcal{B}_n , $g_u : x \mapsto \sum_{j=1}^m \langle x, \psi_j \rangle^{\otimes n} \langle u, \psi_j \rangle^{\otimes n}$, we get

$$\zeta^2(\bar{\varepsilon}) = \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n g_u(v_i) \right]^2.$$

Now, we rely on [Baraud \(2000, Theorem 5.2\)](#) and we write for all $t > 0$,

$$\begin{aligned} \mathbb{P}(\zeta(\bar{\varepsilon}) \geq \mathbb{E}[\zeta(\bar{\varepsilon})] + t) &\leq t^{-p} \mathbb{E}|\zeta(\bar{\varepsilon}) - \mathbb{E}[\zeta(\bar{\varepsilon})]|^p \\ &\leq C(p)t^{-p} \left(\mathbb{E}_1 + \mathbb{E}_2^{p/2} \right), \end{aligned} \tag{45}$$

where \mathbb{E}_1 and \mathbb{E}_2 are defined as

$$\mathbb{E}_1 = \mathbb{E} \left[\max_{i=1, \dots, n} \sup_{u \in \mathcal{B}_n} |g_u(v_i)|^p \right] \quad \text{and} \quad \mathbb{E}_2 = \mathbb{E} \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n g_u^2(v_i) \right].$$

By Cauchy-Schwarz, it is quite straightforward to see that

$$\begin{aligned}\mathbb{E}_1 &= \mathbb{E} \left[\max_{i=1, \dots, n} \sup_{u \in \mathcal{B}_n} \left| \sum_{j=1}^m \langle \varepsilon_i, \psi_{j,i} \rangle \langle u, \psi_j \rangle^{\otimes n} \right|^p \right] \\ &\leq \mathbb{E} \left[\sum_{i=1}^n \|\varepsilon_i\|^p \sup_{u \in \mathcal{B}_n} \left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^p \right],\end{aligned}$$

where $\psi_j = (\psi_{j,1}, \dots, \psi_{j,n})$ for all j in $\{1, \dots, m\}$. Notice that, $\left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^2 \leq 1$ for all u in \mathcal{B}_n and i in $\{1, \dots, n\}$. This leads to

$$\begin{aligned}\mathbb{E}_1 &\leq \tau_p \times \sum_{i=1}^n \sup_{u \in \mathcal{B}_n} \left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^2 \\ &\leq \tau_p \times \sum_{i=1}^n \sup_{u \in \mathcal{B}_n} \left\{ \sum_{l=1}^m |\langle u, \psi_l \rangle^{\otimes n}|^2 \sum_{j=1}^m \|\psi_{j,i}\|^2 \right\} \\ &\leq \tau_p \times \sum_{i=1}^n \sum_{j=1}^m \|\psi_{j,i}\|^2 \\ &\leq m\tau_p.\end{aligned}\tag{46}$$

To upper bound \mathbb{E}_2 , we start with

$$\begin{aligned}\mathbb{E}_2 &= \mathbb{E} \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n \left| \sum_{j=1}^m \langle \varepsilon_i, \psi_{j,i} \rangle^{\otimes n} \langle u, \psi_j \rangle^{\otimes n} \right|^2 \right] \\ &\leq \mathbb{E} \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n \|\varepsilon_i\|^2 \left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^2 \right] \\ &\leq \mathbb{E}_{2,1} + \mathbb{E}_{2,2},\end{aligned}\tag{47}$$

where $\mathbb{E}_{2,1}$ and $\mathbb{E}_{2,2}$ are defined below

$$\begin{aligned}\mathbb{E}_{2,1} &= \mathbb{E} \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n \|\varepsilon_i\|^2 \left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^2 \mathbf{1}_{\|\varepsilon_i\| \leq c} \right], \\ \mathbb{E}_{2,2} &= \mathbb{E} \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n \|\varepsilon_i\|^2 \left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^2 \mathbf{1}_{\|\varepsilon_i\| > c} \right],\end{aligned}$$

with $c > 0$ will be set latter. It is clear that

$$\mathbb{E}_{2,1} \leq c^2.\tag{48}$$

On the flip side,

$$\begin{aligned}\mathbb{E}_{2,2} &\leq c^{2-p} \times \mathbb{E} \left[\sup_{u \in \mathcal{B}_n} \sum_{i=1}^n \|\varepsilon_i\|^p \left\| \sum_{j=1}^m \langle u, \psi_j \rangle^{\otimes n} \psi_{j,i} \right\|^2 \right] \\ &\leq c^{2-p} m\tau_p,\end{aligned}\tag{49}$$

where the last inequality holds with the same arguments when upper bounding \mathbb{E}_1 . Taking $c^p = m\tau_p$ and combining Equations (47), (48) and (49) yields

$$\mathbb{E}_2^{p/2} \leq m\tau_p.\tag{50}$$

From Equations (45), (46) and (50), we get for all $t > 0$ that

$$\mathbb{P}(\zeta(\bar{\varepsilon}) \geq \mathbb{E}[\zeta(\bar{\varepsilon})] + t) \leq C(p)m\tau_p/t^p.$$

Now, the well-known inequality $\mathbb{E}[\zeta(\bar{\varepsilon})]^2 \leq \mathbb{E}[\zeta^2(\bar{\varepsilon})]$ gives

$$\mathbb{P}\left(\zeta^2(\bar{\varepsilon}) \geq \mathbb{E}[\zeta^2(\bar{\varepsilon})] + 2\sqrt{\mathbb{E}[\zeta^2(\bar{\varepsilon})]t^2} + t^2\right) \leq C(p)m\tau_p/t^p.$$

Starting from the last inequality, showing that $\mathbb{E}[\zeta^2(\bar{\varepsilon})] \leq m\sigma_\varepsilon^2$ and taking $t^2 = x$ ends the proof. Indeed, knowing that the $(\varepsilon_i)_i$ are independent and centered, we have

$$\begin{aligned} \mathbb{E}[\zeta^2(\bar{\varepsilon})] &= \sum_{j=1}^m \mathbb{E}\left[\left(\sum_{i=1}^n \langle \varepsilon_i, \psi_{j,i} \rangle\right)^2\right] \\ &\leq \sum_{j=1}^m \sum_{i=1}^n \mathbb{E}\langle \varepsilon_i, \psi_{j,i} \rangle^2 \\ &\leq m\sigma_\varepsilon^2, \end{aligned}$$

where the last upper-bound stems from Cauchy-Schwarz inequality.

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