

# FLAME: Simultaneous variable selection and smoothing for high-dimensional function-on-scalar regression

Alice Parodi <sup>\*</sup>

Matthew Reimherr <sup>†</sup>

Politecnico di Milano

Pennsylvania State University

## Abstract

We present a new methodology, called *FLAME*, which simultaneously selects important predictors and produces smooth estimates in a function-on-scalar linear model with a large number of scalar predictors. To achieve this, the parameters are assumed to be elements of a Hilbert space,  $\mathbb{K}$ , which is different from the space of the data,  $\mathbb{H}$ . We take  $\mathbb{K}$  to be a Reproducing Kernel Hilbert Space, RKHS, which allows us to tune the resulting smoothness of the parameter estimates or incorporate some particular structure, such as periodicity, without enforcing such structures on the data. Our model is fit using a form of penalized functional least squares, which induces both sparsity and smoothness in the resulting estimates. We provide a very fast algorithm for computing the estimators, which is based on a functional coordinate descent, and an R package, `flm`, whose backend is written in C++. Asymptotic properties of the estimators are developed and simulations are provided to illustrate the advantages of FLAME over existing methods, both in terms of statistical performance and computational efficiency. We conclude with an application to childhood asthma, where we find a potentially important genetic mutation that was not selected by previous functional data based methods.

## 1 Introduction

High-dimensional regression and functional data analysis are currently central research areas in statistics and machine learning. The rising interest in both areas reflects the difficult re-

---

<sup>\*</sup>MOX - Department of Mathematics, Politecnico di Milano, Piazza Leonardo da Vinci, 32, Milano, Italy.

<sup>†</sup>Department of Statistics, The Pennsylvania State University, 411 Thomas Building, University Park, PA 16802, USA.

alities of “big data” that many scientists are now facing in their work. Increasingly complex studies and data gathering technologies require sophisticated methods which are mathematically sound, computationally efficient, and practically interpretable. This work concerns a new approach for function-on-scalar regression when the number of predictors is much larger than the number of statistical units. Such data is especially motivated by genetic studies where one encounters large numbers of scalar predictors. These studies are also now increasingly likely to contain sophisticated phenotypic measurements that are suitable for functional data analysis. Our methodology simultaneously exploits the smoothness of the underlying data and functional parameters, as well as the sparsity of the genetic effects. For short, we call this framework *FLAME*, for *functional linear adaptive mixed estimation*. The “mixed” here refers to the mixing of functional norms to simultaneously select significant predictors and smooth their corresponding effect on the functional outcome.

Currently, very little work has been done in this area, but there are several key recent papers which have made substantial in-roads into this problem. For scalar-on-function regression, there are a few recent works (Matsui and Konishi, 2011; Lian, 2013; Gertheiss et al., 2013; Fan et al., 2015), but this is the opposite of the problem we consider here. For function-on-scalar regression, Chen et al. (2016) proposed combining functional least squares with a sparsity inducing penalty. There they took the penalty to be the *group minimax concave penalty*, MCP (Zhang, 2010). In addition, the authors used a pre-whitening technique to more fully exploit the within curve dependence. Unfortunately, the method is computationally expensive and cannot be applied when the number of predictors,  $I$ , is greater than the sample size,  $N$ , meaning that it cannot be applied to our intended high-dimensional applications. As we shall see in Section 5.2.2, the pre-whitening can also be counter productive when working with densely sampled functional data. Barber et al. (2016) proposed the function-on-scalar lasso, FSL, which uses penalized functional least squares. In their approach they assumed the data and parameters were from an arbitrary Hilbert space, but to induce sparsity, the penalty was taken to be a type of induced  $\ell_1$  norm on the product space

of Hilbert spaces where the parameters and data lie. Their approach is computationally efficient since it is a convex optimization problem, and achieves optimal rates of convergence for the parameter estimates even when the number of predictors,  $I$ , is much larger than the sample size  $N$  ( $I \gg N$ ). However, the method, like traditional lasso, does not achieve the functional oracle property due to a non-negligible asymptotic bias. To that end, in a follow up paper Fan and Reimherr (2016) developed an adaptive version, AFSL, and showed it achieves, what we call here, the *strong functional oracle property*, which we will discuss in further detail in Section 4. Furthermore, this method can be implemented at nearly the same computational cost as FSL.

The major contributions of this work are as follows. We develop a new high-dimensional functional regression methodology that simultaneously selects important predictors and provides smooth estimates of their effects; previous approaches focussed on selection only. Using convex analysis over Hilbert spaces, we provide a coordinate descent algorithm for model fitting and a very fast R package, `flm`, whose backend is written C++; previous methods “piggybacked” off of existing multivariate tools while ours is customized for functional data, resulting in substantial gains in computational efficiency. As part of this computational efficiency, we also avoid the use of the “Representer Theorem” of RKHSs for expressing parameter estimates, which, while theoretically convenient, is often not computationally efficient (Sriperumbudur and Szabó, 2015). Instead we utilize the eigenfunctions of the kernel to expand the parameters, which can dramatically improve computational efficiency. We also provide asymptotic theory, which demonstrates that FLAME achieves a functional version of the oracle property. This theory requires substantial advances over the theory for FS-LASSO as we are mixing Hilbert space and RKHS norms, which are not equivalent (in a mathematical sense). Lastly, our framework allows one to build in a variety of structures into the parameters, including smoothness and periodicity. As can be seen in Section 5 this can result in dramatic gains in statistical efficiency.

The paper is organized as follows. In Section 2 we outline several important concepts

from FDA as well as the modeling assumptions of the data. In Section 3 we detail our approach, presenting a coordinate descent algorithm which allows FLAME to be computed very efficiently. In Section 4 we present asymptotic theory, and in Sections 5 we present numerical illustrations including simulations and an application to a longitudinal genetic association study.

## 2 Background and Methodology

For a detailed introduction to FDA we refer the interested reader to Ramsay and Silverman (2006); Graves et al. (2009); Horváth and Kokoszka (2012); Hsing and Eubank (2015); Kokoszka and Reimherr (2017). For an introduction on machine learning and high dimensional regression we refer the reader to Hastie et al. (2001); Bühlmann et al. (2010); James et al. (2013); Hastie et al. (2015). Let  $\mathbb{H}$  be a real separable Hilbert space, with norm  $\|\cdot\|_{\mathbb{H}}$ ; our theory will hold quite generally for data from an arbitrary real separable Hilbert space. In this way, our methodology is quite broad covering typical spaces such as  $L^2[0, 1]$ , as well as product spaces, Sobolev spaces, etc. Let  $K$  be a compact linear operator from  $\mathbb{H} \rightarrow \mathbb{H}$ . We assume that it is positive definite and self-adjoint:

$$\langle Kx, x \rangle \geq 0 \quad \langle Kx, y \rangle = \langle x, Ky \rangle.$$

The spectral theorem (Dunford and Schwartz, 1963) implies that we can decompose  $K$  as

$$K = \sum_{i=1}^{\infty} \theta_i v_i \otimes v_i,$$

where  $\theta_1 \geq \theta_2 \geq \dots \geq 0$  are the ordered eigenvalues and  $v_i \in \mathbb{H}$  are the corresponding eigenfunctions. The eigenfunctions  $\{v_i\}$  form an orthonormal basis in  $\mathbb{H}$ . The tensor product  $x \otimes y$  is used to denote the operator  $(x \otimes y)(h) := \langle y, h \rangle x$ . We define a subspace of  $\mathbb{H}$ , denoted

$\mathbb{K}$ , as follows:

$$\mathbb{K} := \left\{ h \in \mathbb{H} : \sum_{i=1}^{\infty} \frac{\langle h, v_i \rangle^2}{\theta_i} = \langle K^{-1}h, h \rangle < \infty \right\}.$$

If we equip  $\mathbb{K}$  with the norm  $\|h\|_{\mathbb{K}} = \|K^{-1/2}h\|_{\mathbb{H}}$  then this space also a Hilbert space. Here it is understood that  $0/0 = 0$ . When  $\mathbb{H}$  is  $L^2[0, 1]$  and the kernel of  $K$  is a bivariate function, i.e.  $K(t, s)$ , then  $\mathbb{K}$  is also a reproducing kernel Hilbert space (Berlinet and Thomas-Agnan, 2011).

We now make the following modeling assumption about the response functions,  $Y_n \in \mathbb{H}$ , and the predictors  $X_{n,i} \in \mathbb{R}$ .

**Assumption 1** *Let  $Y_1, \dots, Y_N$  be elements of  $\mathbb{H}$ , satisfying the functional linear model*

$$Y_n = \sum_{i=1}^I X_{n,i} \beta_i^* + \varepsilon_n,$$

where  $\mathbf{X} = \{X_{n,i}\} \in \mathbb{R}^{N \times I}$  is the deterministic design matrix with standardized columns, and  $\varepsilon_n$  are i.i.d. Gaussian random elements of  $\mathbb{H}$  with mean function 0 and covariance operator  $C$ . We assume that there exists  $0 \leq I_0 \leq I$  such that only  $\beta_1^*, \dots, \beta_{I_0}^*$  are nonzero. This means that, for notational simplicity, the first  $I_0$  of the predictors are significant in the model. We will use the notation  $\mathbf{X} = (\mathbf{X}_1 \ \mathbf{X}_2)$  to partition the predictors into the significant predictors,  $\mathbf{X}_1$ , and the null predictors  $\mathbf{X}_2$ .

Note that any Gaussian process in  $\mathbb{H}$  will necessarily have a mean function in  $\mathbb{H}$  and a covariance operator  $C$  which is compact, symmetric, and positive definite (Laha and Rohatgi, 1979). In our theory, the normality is only used to derive functional concentration inequalities. These inequalities determine the rate at which  $I$  can grow with  $N$ . When the errors are Gaussian, one has that  $I$  can grow exponentially fast relative to  $N$ , and the assumptions (as given in Assumption 2) are easier to interpret. Our arguments can be readily generalized to the non-normal case, but the rates will change and the assumptions will be more complicated, we thus do not pursue that direction presently.

The FLAME target function is given by

$$L(\beta) = \frac{1}{2N} \sum_{n=1}^N \|Y_n - X_n^\top \beta\|_{\mathbb{H}}^2 + \lambda \sum_{i=1}^I \tilde{\omega}_i \|\beta_i\|_{\mathbb{K}} = \frac{1}{2N} \|Y - \mathbf{X}\beta\|_{\mathbb{H}}^2 + \lambda \sum_{i=1}^I \tilde{\omega}_i \|\beta_i\|_{\mathbb{K}},$$

with  $Y \in \mathbb{H}^N$ ,  $\mathbf{X} \in \mathbb{R}^{N \times I}$  and  $X_n = \mathbf{X}_{(n,\cdot)} \in \mathbb{R}^I$ ,  $\beta \in \mathbb{K}^I$ . Throughout, we use notation such as  $\mathbb{H}^N$  to denote product spaces. For the sake of simplicity, we abuse notation a bit by letting  $\|\cdot\|_{\mathbb{H}}$  also denote the induced Hilbert space norm on product spaces such as  $\mathbb{H}^N$ . There are at least a few data driven ways one can choose the weights  $\tilde{\omega}_i$ . One option is to use marginal regressions to get initial parameter estimates, then the weights would be one over the norms of those estimates (Huang et al., 2008). Another option is to run FSL first and then use its corresponding estimates. This has the advantage of also dramatically reducing the dimension of the problem, and is the approach we take for developing our asymptotic theory in Section 4. Lastly, one could first run the nonadaptive version of FLAME (i.e. with  $\tilde{\omega} \equiv 1$ ) to obtain preliminary estimates,  $\tilde{\beta}_i$ , and then compute the weights as  $\tilde{\omega}_i = \|\tilde{\beta}_{i,N}\|_{\mathbb{K}}^{-1}$ . This is the approach we take for our empirical work in Section 5. Our reasoning is that we wanted a more pure comparison between the different methods to compare their performances. Since all of the methods, except FSL, utilize a preliminary run to different degrees, opening the door to mixing and matching would create a huge number of potential options, and is beyond the scope of this paper.

In our approach we use the norm  $\|\cdot\|_{\mathbb{K}}$  to both induce sparsity and smooth the parameter estimates. Previous approaches have focused only on one or the other. Furthermore, by allowing for a general  $K$ , we provide a framework which is very flexible and can accommodate a variety of underlying assumptions about the parameters, such as periodicity and boundary conditions. The purpose of the data driven weights is to penalize “smaller” parameters more, and thus not shrink the larger ones as much. This allows the estimator to be asymptotically unbiased and achieve an oracle property. We now discuss several examples of popular kernels.

**Example 1 (Sobolev Space)** Consider  $\mathbb{H} = L^2(\mathcal{D})$ , where  $\mathcal{D}$  is a compact subset of  $\mathbb{R}^d$ .

Define  $\mathbb{K}$  to be the subset of functions in  $L^2(\mathcal{D})$  that have up to and including  $m^{\text{th}}$  order derivatives that are also in  $L^2(\mathcal{D})$ . A family of norms can be defined on  $\mathbb{K}$  as

$$\|x\|_{\mathbb{K}}^2 = \sum_{|\alpha| \leq m} \frac{1}{\sigma_{\alpha}^2} \int_{\mathcal{D}} |x^{(\alpha)}(\mathbf{s})|^2 d\mathbf{s}.$$

Here  $\alpha$  is a  $d$ -dimensional vector of integers whose sum is less than or equal to  $m$ , while the  $\sigma_{\alpha}$  are nonzero weights. Equipped with this norm,  $\mathbb{K}$  is an RKHS if and only if  $m > d/2$ . In the case where  $\mathcal{D} = [0, 1]$  and  $m = 1$ , we have that

$$K(t, s) = \begin{cases} \frac{\sigma}{\sinh(\sigma)} \cosh(\sigma(1-s)) \cosh(\sigma t) & t \leq s \\ \frac{\sigma}{\sinh(\sigma)} \cosh(\sigma(1-t)) \cosh(\sigma s) & t > s \end{cases}.$$

One can then numerically solve for the eigenfunctions and eigenvalues of  $K$ . These details can be found on Page 281 of Berlinet and Thomas-Agnan (2011).

**Example 2 (Gaussian Kernel)** Let  $\mathbb{H} = L^2(\mathcal{D})$ , then the Gaussian kernel is given by

$$K(\mathbf{s}, \mathbf{s}') = \exp \{ -\sigma |\mathbf{s} - \mathbf{s}'|^2 \}.$$

While the Sobolev spaces contain functions which are differentiable up to a given order, the space  $\mathbb{K}$  here contains functions which are infinitely differentiable. When used in FLAME, such a kernel will produce very smooth estimates.

**Example 3 (Exponential Kernel)** The exponential kernel is on the other end of the “smoothness” spectrum compared to the Gaussian kernel. In this case we have

$$K(\mathbf{s}, \mathbf{s}') = \exp \{ -\sigma |\mathbf{s} - \mathbf{s}'| \}.$$

This seemingly minor adjustment to the power in the exponent produces a space consisting of continuous functions which need not be differentiable. Using this kernel will produce

substantially rougher FLAME estimates than the Gaussian kernel. In practice, they will be a bit rougher than the Sobolev kernel as well.

**Example 4 (Periodic Kernel)** *A very useful feature of working with an RKHS is that one can incorporate structures such as periodicity and boundary conditions into the parameter estimates. This may be useful, for example, when the domain represents time over the course of a year. In that case, one might expect the parameters to be periodic. In this case one may use the periodic kernel with period  $p = 1$  for yearly periodicity,  $p = 1/2$  for semestral periodicity, or  $p = 1/4$  for seasonal. The periodic kernel with period  $p$  is defined as*

$$K(\mathbf{s}, \mathbf{s}') = \sigma^2 \exp \left\{ -2/\sigma \sin^2 \left( \frac{\pi |\mathbf{s} - \mathbf{s}'|}{p} \right) \right\}.$$

*More general boundary conditions can be worked into Sobolev spaces and norms, but we refrain from printing the details here, since we will not explore them in our simulations. An interested reader is referred to, for example, Section 4 of Chapter 7 in Berlinet and Thomas-Agnan (2011) who list many examples of kernels that can work in different structures.*

### 3 Implementation and computational details

In this section we develop a coordinate descent algorithm for quickly finding the FLAME estimator. These methods are implemented in an accompanying R package `flm`. The computationally intensive functions in this package are coded in C++, so that the methodology can be implemented very quickly even for very large datasets.

The algorithm is based on utilizing functional subgradients so that, at each step, individual parameter estimates can be updated very quickly in a nearly closed form. An interested reader is referred to Boyd and Vandenberghe (2004); Bauschke and Combettes (2011); Barbu and Precupanu (2012); Shor (2012) for more details on subgradients and subdifferentials. Subgradients generalize derivatives (in this case Fréchet derivatives) to convex functionals (mappings from  $\mathbb{H}$  to  $\mathbb{R}$ ) which are not necessarily differentiable. At any point where the

functional is differentiable, the two notions coincide, but subgradients are well defined much more broadly to convex functionals that need not be differentiable. Let  $f : \mathbb{H} \rightarrow \mathbb{R}$  be a convex functional. We say that  $h \in \mathbb{H}$  is a subgradient of  $f$  at  $x \in \mathbb{H}$  if for all  $y \in \mathbb{H}$  we have

$$f(x + y) - f(x) \geq \langle h, y \rangle.$$

We denote by  $\partial f(x)$  the collection of all subgradients of  $f$  at  $x$ , called the subdifferential. Trivially,  $x$  is a minimizer of  $f$  if and only if  $0 \in \partial f(x)$ . We show in the supplemental material that the subgradient for FLAME is given by

$$(1) \quad \frac{\partial}{\partial \beta_i} L_\lambda(\beta) = -\frac{1}{N} \sum_{n=1}^N X_{n,i} K(Y_n - X_n^\top \beta) + \lambda \tilde{\omega}_i \begin{cases} \|\beta_i\|_{\mathbb{K}}^{-1} \beta_i, & \beta_i \neq 0 \\ \{h \in \mathbb{K} : \|h\|_{\mathbb{K}} \leq 1\}, & \beta_i = 0 \end{cases}.$$

At each step of the coordinate descent we can use (1) to update our estimates. In particular, suppose that  $\hat{\beta}$  is our current estimate and we aim to update the  $i^{\text{th}}$  coordinate,  $\hat{\beta}_i$ . The least squares estimator would be

$$\check{\beta}_i = \frac{1}{N} \sum_{n=1}^N X_{n,i} E_n \quad \text{where} \quad E_n = Y_n - \sum_{j \neq i} X_{n,j} \hat{\beta}_j.$$

We can then express the subgradient as

$$\frac{\partial}{\partial \beta_i} L(\beta) = -K(\check{\beta}) + K(\beta_i) + \lambda \omega_i \begin{cases} \|\beta_i\|_{\mathbb{K}}^{-1} \beta_i, & \beta_i \neq 0 \\ \{h \in \mathbb{K} : \|h\|_{\mathbb{K}} \leq 1\}, & \beta_i = 0 \end{cases}.$$

We can immediately observe that

$$(2) \quad \|K(\check{\beta}_i)\|_{\mathbb{K}} \leq \lambda \omega_i \implies \hat{\beta}_i = 0.$$

Note this also indicates a useful starting value of  $\lambda$  for the algorithm; if we take

$$(3) \quad \lambda = \max_{i=1,\dots,I} \{\omega_i^{-1} \|N^{-1} \sum X_{ni} K(Y_n)\|_{\mathbb{K}}\},$$

then the solution will always be  $\hat{\beta}_i = 0$ . When  $\hat{\beta}_i \neq 0$ , we can solve for it in a nearly closed form. In particular, we have

$$(4) \quad -K(\check{\beta}_i) + K(\hat{\beta}_i) + \frac{\lambda\omega_i}{\|\hat{\beta}_i\|_{\mathbb{K}}} \hat{\beta}_i = 0 \implies \hat{\beta}_i = \left( K + \frac{\lambda\omega_i}{\|\hat{\beta}_i\|_{\mathbb{K}}} I \right)^{-1} K(\check{\beta}_i).$$

The only unknown quantity at this point is  $\|\hat{\beta}_i\|_{\mathbb{K}}$ . Unfortunately, its expression does not have a closed form solution (unlike FLS or AFSL). However, if we take the  $\mathbb{K}$ -norm of the expression in (4) we arrive at the following equation that can be solved numerically

$$1 = \sum_{j=1}^{\infty} \frac{\theta_j \langle \check{\beta}_i, v_j \rangle^2}{(\theta_j \|\hat{\beta}_i\|_{\mathbb{K}} + \lambda\omega_i)^2}.$$

Our coordinate descent algorithm therefore proceeds iteratively, defining a sequence of  $\beta^{(t)}$  for  $t = 1, \dots, T$  which converges to the desired approximation  $\hat{\beta}$ . We set the maximum number of iterations  $T$  and a stopping criteria based on the improvement in the estimation of the  $\beta$  coefficients (i.e. the  $\mathbb{K}$ -norm of the increment should be higher than a fixed tolerance).

Regarding the weights,  $\tilde{\omega}_i$ , we run the algorithm twice. The first one (*the non-adaptive step*) is run with weights set to 1, and the second time (*adaptive step*) we take  $\tilde{\omega}_j = \|\hat{\beta}_{j,N}\|_{\mathbb{K}}^{-1}$  with  $\|\hat{\beta}_{j,N}\|_{\mathbb{K}}$  the norm of the  $\beta$  estimated in the *non-adaptive step*. In particular the *adaptive step* is run to improve the estimation of the meaningful predictors and then the algorithm is run only on the non-zero predictors isolated in the *non-adaptive step*. These steps must be run for a sequence of  $\lambda$  and we have to identify a proper  $\lambda$  which maximizes some selection criterion; we choose  $\lambda$  to minimize the cross validation error, once we have isolated a training and a test set (randomly sampled as the 25% of the whole data set).

We mention two features we have built into the code which help increase its computational

efficiency. The first is a *warm start* which means when moving to the next  $\lambda$  value, we use the previous  $\hat{\beta}$  as the initial value for  $\beta$ . Since  $\lambda$  usually changes very little with each step, this means that the new  $\hat{\beta}$  can be computed very quickly (usually with just a few iterations). In this way, one can obtain the solutions for an entire sequence of  $\lambda$  with only marginally more computation time than with a single  $\lambda$ . The second feature is what we call a *kill switch*. This allows the user to set the maximum size for the number of predictors selected by the model. When the algorithm moves past this threshold, the algorithm is stopped. In certain applications, one can make a good guess as to the maximum number of predictors that could conceivably be selected by the model. In these settings, this bound can be used for the *kill switch*. For example, in genetic studies, even with hundreds of thousands of predictors, it is usually safe to assume that far fewer than say 100 SNPs, will actually be selected (usually the number is far less than 100). The algorithm slows down as more predictors enter the model, thus this has the potential to provide a substantial computational savings.

Lastly, all functional data methods of this type require some preprocessing of the raw data into functional units. This is now a fairly well developed step and a more detailed discussion can be found in Horváth and Kokoszka (2012). In short, we utilize a penalized cubic bsplines expansion, where the penalty is chosen by generalized cross validation. The number of bsplines in our simulations and application is taken to be 100 so that the smoothing is determined entirely by the penalty. In FSL and AFSL one would then commonly rotate to the FPCA basis so that less than 100 basis functions can be used, thus gaining computational efficiency. For FLAME, we instead use the eigenfunctions of the kernel  $K$ , which we compute numerically on a fine grid. This allows us to quickly compute both  $\mathbb{H}$  norms and  $\mathbb{K}$  norms. We choose the number of basis functions,  $J$ , so that

$$\sum_{j=1}^J \theta_j \geq 0.99 \sum_{j=1}^{\infty} \theta_j,$$

where  $\theta_j$  are the eigenvalues of the kernel  $K$ . This formulation is similar to explaining 99%

of the variability in FPCA. We use such a high mark because dimension reduction is not our goal; we aim to approximate the data nearly exactly.

## 4 Theoretical Properties

In this section we provide several theoretical guarantees for FLAME. While this theory provides a strong justification for using FLAME, there are still several interesting theoretical questions which remain open and will be discussed below. We begin by making the following assumption concerning the various terms in the model. Very similar assumptions can also be found in Fan and Reimherr (2016).

**Assumption 2** *The regression problem satisfies the following.*

1. **Minimum Signal:** Let  $b_N = \min_{i \in \mathcal{S}} \|K(\beta_i^*)\|_{\mathbb{K}}$ , then we assume the lower bounded

$$b_N^2 \gg \frac{I_0^2 \log(I)}{N}.$$

2. **Tuning Parameter:** The tuning parameter  $\lambda$  satisfies the following lower and upper bounds

$$\frac{I_0^{1/2} \log(I)}{N} \ll \lambda \ll \frac{b_N}{\sqrt{I_0} \sqrt{N}}.$$

3. **Design Matrix:** Let  $\hat{\Sigma}_{11} = N^{-1} \mathbf{X}_1^\top \mathbf{X}_1$ , be the design matrix for only the true predictors. We assume the minimum eigenvalue  $\sigma_{\min}(\hat{\Sigma}_{11})$  and maximum eigenvalue  $\sigma_{\max}(\hat{\Sigma}_{11})$  satisfy:

$$\frac{1}{\nu_1} \leq \sigma_{\min}(\hat{\Sigma}_{11}) \leq \sigma_{\max}(\hat{\Sigma}_{11}) \leq \nu_1.$$

4. **Irrepresentable Condition** Let  $\hat{\Sigma}_{21} = N^{-1} \mathbf{X}_2^\top \mathbf{X}_1$ , be the cross covariance between the null and true predictors. We assume that

$$\|\hat{\Sigma}_{21} \hat{\Sigma}_{11}^{-1}\|_{op} \leq \phi < 1$$

with  $\phi$  a fixed scalar and  $\|\cdot\|_{op}$  the operator norm.

The first assumption is called a minimum signal condition and indicates the minimum magnitude (of the signals) required for detecting the relevant predictors. Notice that this condition is placed on  $\beta^*$  relative to  $K$ , which means that if  $K$  wipes out a signal, the algorithm will not be able to detect it. The second condition concerns the rate for  $\lambda$ , and takes a fairly familiar form (Barber et al., 2016; Fan and Reimherr, 2016). Since our FLAME formulation normalizes the sum of squares by  $N$ , the  $\lambda$  needs to tend to zero. The lower bound, indicates that it cannot go to zero too quickly, otherwise one cannot guarantee that all of the null predictors are dropped. Conversely, the upper bound actually indicates two things, first if  $\lambda$  goes to zero too slowly then some of the significant predictors may also be dropped. Second, the upper bound on  $\lambda$  also ensures the bias is asymptotically negligible for establishing an oracle property. The third condition on the design matrix simply says that the design matrix for the true predictors, must be well behaved. This ensures that the oracle estimate as well as the FLAME estimate are well behaved when restricted to the set of true predictors. The last condition is interpreted as requiring that the true predictors and the null predictors are not too correlated. This condition is essentially necessary to obtain an oracle property (Zhao and Yu, 2006).

Under these conditions, we can now state our primary theorem, which states that FLAME recovers the true support with probability tending to 1, and that its projections are asymptotically normal.

**Theorem 1** *If the regression problem satisfies Assumptions 1 and 2, the solution of the FLAME problem,  $\hat{\beta}$ , asymptotically*

1. *has the same support of the true solution of the regression problem*

$$P(\hat{\beta} \stackrel{S}{=} \beta^*) \rightarrow 1,$$

2. *and is equivalent to the Oracle estimator in the sense that, for any sequence  $h_n =$*

$\{h_{i,n}\} \in \mathbb{K}^I$  that satisfies  $\|h_n\|_{\mathbb{K}} \leq M_1$  and  $\sum \|C^{1/2}h_{i,n}\|_{\mathbb{H}}^2 \geq M_2 > 0$  we have

$$\frac{\sqrt{N}\langle \hat{\beta} - \beta^*, h_n \rangle}{\sigma_n} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1) \quad \text{where} \quad \sigma_n^2 = \sum_{i \in \mathcal{S}} \sum_{j \in \mathcal{S}} \hat{\Sigma}_{11;ij}^{-1} \langle C^{1/2}h_i, C^{1/2}h_j \rangle.$$

The first part of the theorem is a fairly standard result; we are showing that our method is variable selection consistent. The second result shows that the estimators are consistent and are asymptotically normal, but there is a serious caveats to this, namely the projections are normal only when projected onto an element of  $\mathbb{K}$ , not  $\mathbb{H}$ . If the  $Y_n$  were finite dimensional, then the two would be equivalent, but not in the functional setting.

In the context of functional data, we call Theorem 1 a *weak oracle property* because the normality occurs in the weak topology (i.e. on projections). Such results are not uncommon in functional data analysis (Cardot et al., 2007). Our next result shows that one can actually obtain a stronger result, namely, that the FLAME and oracle estimates are asymptotically equivalent in the *strong* topology. For this reason, we say that the following theorem is a *strong oracle property*. First let us define the oracle estimate, namely

$$\hat{\beta}_O = \{(\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top Y, 0\},$$

where 0 a vector of zero functions of length  $I - I_0$ .

**Theorem 2** *Suppose Assumptions 1 and 2 are satisfied, but that  $I_0$  is fixed. Furthermore, assume there exists a  $\delta > 0$  and a constant  $0 < B < \infty$  such that for all  $i \in \mathcal{S}$*

$$\sum_{j=1}^{\infty} \frac{\langle \beta_i^*, v_j \rangle^2}{\theta_j^{1+\delta}} \leq B < \infty.$$

*If  $\lambda$  is such that*

$$\lambda \ll \frac{b_N}{N^{1/2[1+1/(1+\delta)]}},$$

then one also has that

$$\sqrt{N}\|\hat{\beta} - \hat{\beta}_O\|_{\mathbb{H}} = o_P(1).$$

Notice that we have introduced slightly stronger assumptions to achieve a strong oracle property. In particular, we needed a more explicit assumption on the rate at which the coordinates of  $\beta^*$  decrease. If  $\delta = 0$  this simply implies that  $\beta^*$  is in  $\mathbb{K}$ . Lastly, we require a tighter control of the  $\lambda$  which depends on how quickly the coordinates of  $\beta^*$  decrease. If the coordinates actually terminate (i.e. are zero) at a certain point or if they decrease exponentially fast, then our assumption on  $\lambda$  is the same as before. The assumption that  $I_0$  is fixed allows us to simplify the results. Using our techniques it is possible to allow  $I_0$  to grow, but we would need additional assumptions on the behavior of the trace of the covariance operator of the errors with respect to the  $\{v_i\}$  basis, and so do not pursue it here.

We believe that our results can be tightened, especially the additional assumptions needed to achieve Theorem 2. Maybe the major obstacle is obtaining a good control of  $\|\hat{\beta}\|_{\mathbb{K}}$ . This quantity shows up when updating via coordinate descent and when trying to control the bias of the FLAME estimate. However, unlike FSL, we do not have an explicit expression for this quantity in terms of the least squares estimator. If one can obtain a tighter control of this quantity, it should be easier to relax the assumptions of Theorem 2. Lastly, it might be interesting to study the asymptotic properties of  $\hat{\beta}$  under the  $\mathbb{K}$  norm, instead of the  $\mathbb{H}$  norm. For example, it might be of interest to study the estimated derivatives of the parameters. However, since this is a much stronger norm, clearly additional assumptions will be needed. Furthermore, the oracle estimate would not be the least squares estimator as this need not even live in the space  $\mathbb{K}$ . We thus believe there are many open and exciting questions concerning the behaviors of such functional estimators and their necessary assumptions.

## 5 Empirical study

In this section we introduce several simulation schemes to analyze the performances of FLAME with different RKHS (Section 5.1) and to compare this method with AFSL and MCP (Section 5.2). We conclude (Section 5.3) with an application to a large genetic dataset. For all simulations we assume data in  $L^2[0, 1]$ . The kernels we consider are three popular kernels, the Exponential, the Sobolev, and the Gaussian. Moreover, for the specific case of Section 5.2.3 we introduce the periodic kernel. In Figure 1, the first four eigenfunctions associated to the Exponential, the Sobolev, and the Gaussian kernel are plotted and the explained variance is shown. These three kernels show different structure and complexity; in Section 5.1 the consequences of the different smoothness levels required to functions embedded in these kernels are presented.

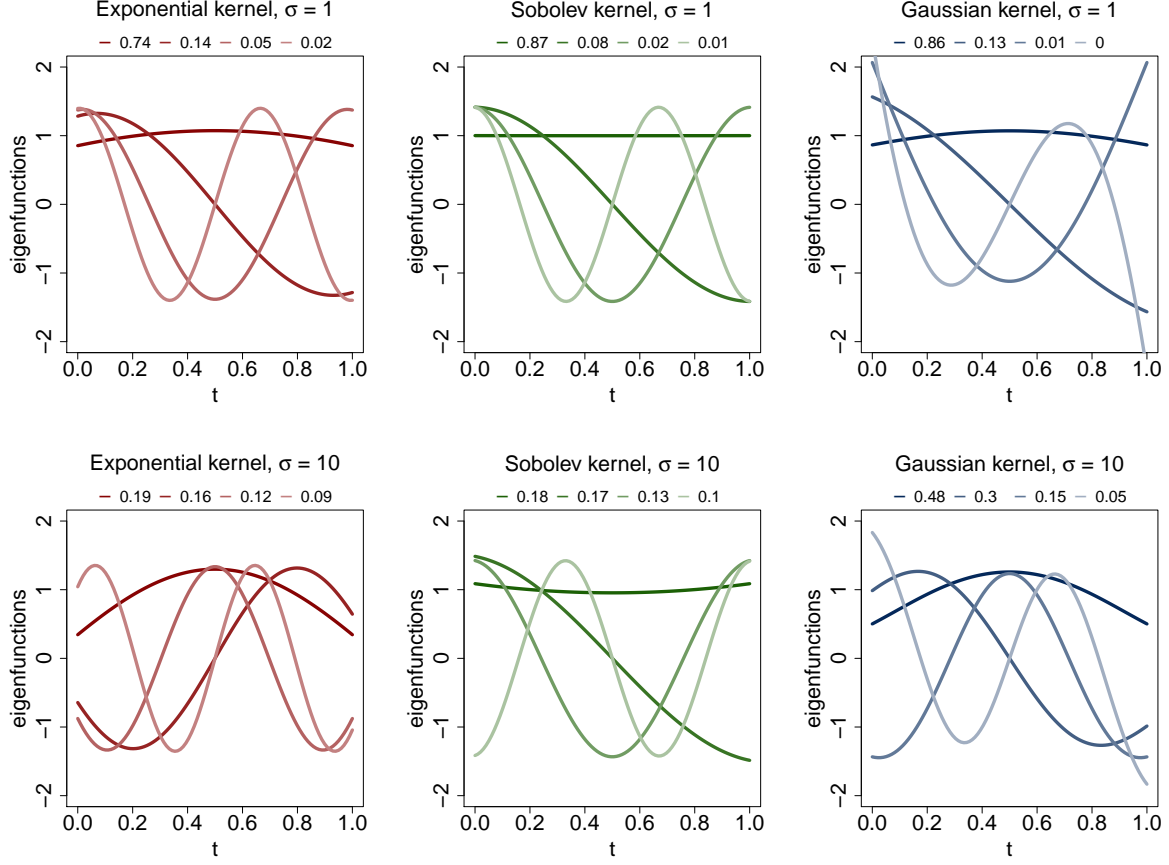
All simulations used 100 runs on a Intel quad-core i7 desktop with 8GB of ram with the vecLib linear algebra library of R and measured in terms of:

- *computational time*: median of the computational time (sec.) of the runs.
- *number of true positive predictors*: average number of correctly non-zero predictors identified (i.e.  $\#\{i : \beta_i^* \neq 0 \wedge \hat{\beta}_i \neq 0\}$ ).
- *number of false positive predictors*: average number of wrongly identified non-zero predictors (i.e.  $\#\{i : \beta_i^* = 0 \wedge \hat{\beta}_i \neq 0\}$ ).
- *prediction error*: average of the prediction error, both for data and derivatives,

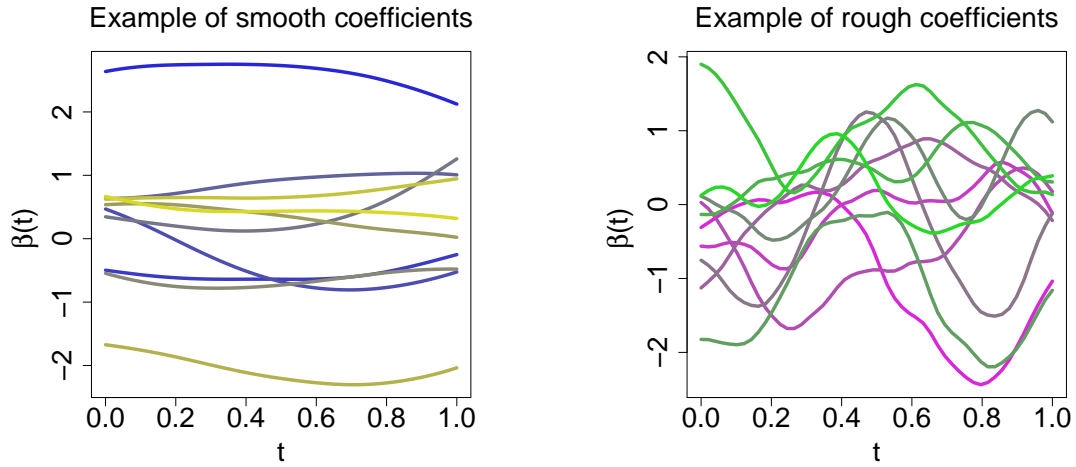
$$\sum_{n=1}^N \| \mathbf{X}_n \beta^* - \mathbf{X}_n \hat{\beta} \|_{L^2} \text{ and } \sum_{n=1}^N \| \mathbf{X}_n \beta^{*\prime} - \mathbf{X}_n \hat{\beta}' \|_{L^2}$$

### 5.1 Comparison between different kernels

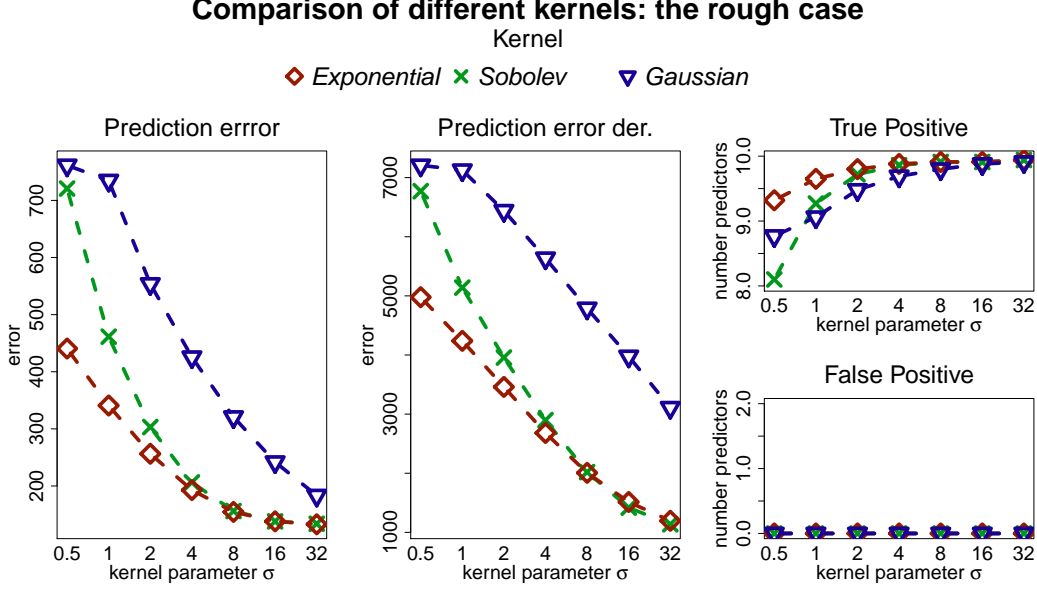
In this section we compare the performance of FLAME using different kernels. We show how the variation of the kernel can influence the identification of the number of correctly



**Figure 1:** Representation of the first four eigenfunctions for each kernel with different  $\sigma$ . From the left: the Exponential, the Sobolev and the Gaussian kernel. The legend at the top of each panel denotes proportion of the explained variability for each eigenfunction.



**Figure 2:** Example of 10  $\beta^*$  coefficients for the smooth (left panel) and rough (right panel) simulation setting.



**Figure 3:** Summary of the simulations varying kernel for the rough case. From the left, the prediction error, the prediction error on derivatives, and the number of true and false positive predictors. We can notice that in all the simulations the number of False Positive estimated predictors is 0. No extra parameters are estimated with FLAME, while the number of True Positive predictors increases with the roughness level of the kernel.

identified predictors and the prediction error. Two high-dimensional simulation settings are introduced: with rough and smooth  $\beta^*$  coefficients.

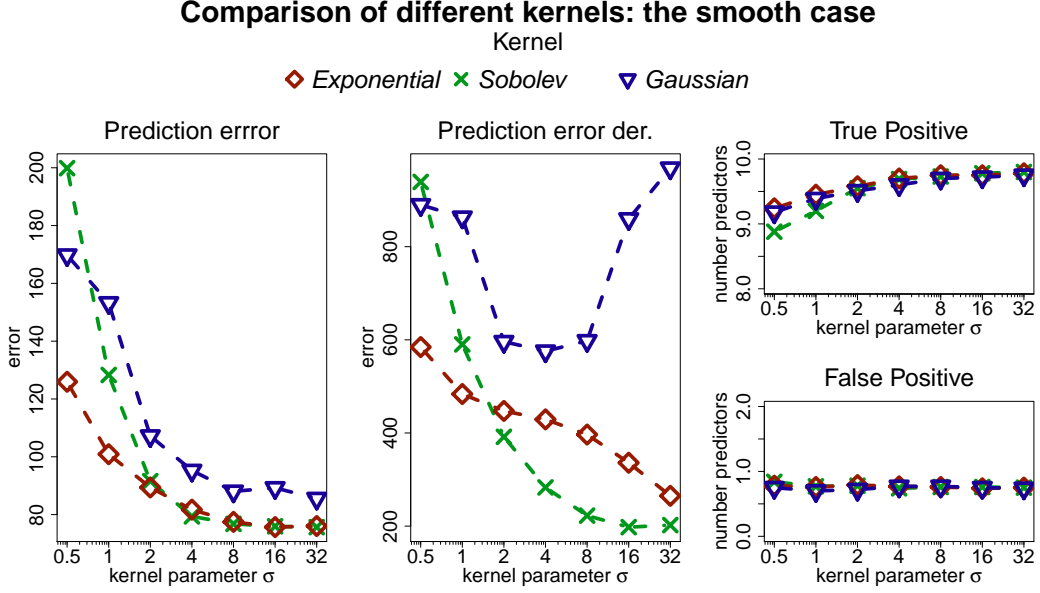
The simulations consist of the random generation of a sample of size  $N = 500$  and  $I = 1000$  predictors, with  $I_0 = 10$  significant ones. The predictor matrix  $\mathbf{X}$  is the standardized version of a matrix randomly sampled from a  $N$  dimension Gaussian distribution with 0 average and covariance  $\Sigma_X = \mathbb{1}$ . For the rough case, the true coefficients  $\beta^*(t)$  are sampled from a Matérn process with 0 average and parameters  $(\nu = 2.5, \text{range} = 1/4, \sigma^2 = 1)$ , while for the smooth setting the range parameter of the Matérn process is set to 1 and  $\nu$  is set to 3.5. In Figure 2 an example of the true coefficients in the two settings is shown. The outcomes,  $Y_n(t)$ , are obtained as the sum of the contribution of all the predictors and a random noise, a 0-mean Matérn process with parameters  $(\nu = 1.5, \text{range} = 1/4, \sigma^2 = 1)$ . Functions are sampled on an evenly spaced grid between 0 and 1 with  $m = 50$  points.

For these simulations the *kill switch* parameter is set to  $2I_0 = 20$  and  $\lambda$  spans a logarithmic equispaced 100-point grid from  $\lambda_{\max}$  of (3) to  $r_\lambda \lambda_{\max}$  with  $r_\lambda = 0.01$  for the rough case and  $r_\lambda = 0.001$  for the smooth setting. A summary of the result is shown in Figure 3 for the rough case and in Figure 4 for the smooth case.

Focusing on the rough setting we notice that the Gaussian kernel always performs worse than other kernels in terms of prediction error both for data and derivatives: it imposes on the functions a structure (infinitely differentiable) they don't possess. Moreover, increasing the  $\sigma$  parameter of the kernels, which results in a rougher estimates, reduces the prediction error and more true non zeros predictors are identified. In fact, with a too strong smoothness level, imposed by the Gaussian kernel or by a small value for the  $\sigma$  parameter, some true predictors are forced to be zero throughout the domain and this reduces the number of true positives and increases the prediction error. The rough structure of the parameters allows to all the methods presented to avoid the identification of non significant predictors and the number of False Positive is always zero.

A slightly different behavior can be observed in the smooth case. The performance of the Gaussian kernel, while still worse, is now much closer in performance to the other two kernels. The strange behavior of the prediction error of derivatives for the gaussian and the exponential kernel is due to an instability in the estimation of the derivatives of the eigenfunctions of these kernels at the boundaries of the time domain (not shown here). The number of False Positive predictors in this setting is different from zero (but it remains on average smaller than one per simulation).

A final remark regarding the high dimensional setting is the computational cost of the estimation and variable selection procedure. As presented in Table 1, the computational time is almost invariant with respect to the kernel and parameter, while increasing the smoothness level of the predictors increases the computational time. In the next section we present how competitive FLAME is compared to different methods.



**Figure 4:** Summary of the simulations varying kernel for the smooth case. From the left, the prediction error, the prediction error on derivatives, and the number of true and false positive predictors.

FLAME				FLAME			
Kernel				Kernel			
$\sigma$	Gaus.	Sob.	Exp.	$\sigma$	Gaus.	Sob.	Exp.
0.5	29.30	30.75	41.14	0.5	80.38	85.81	95.00
1	21.64	36.62	48.17	1	77.67	81.33	94.66
2	28.87	43.92	58.67	2	72.23	87.59	97.95
4	32.34	39.14	61.48	4	66.69	76.18	91.18
8	32.61	42.99	47.29	8	58.46	79.12	99.08
16	33.67	42.59	39.95	16	61.14	80.36	92.98
32	35.47	33.47	40.83	32	63.23	70.22	69.97

**Table 1:** Median time for the simulations varying kernel for the rough (left panel) and smooth case (right panel).

	prediction error	prediction error der.	True Positive	False Positive	Time (sec.)
rough setting	352.51	4664.2	9.92	0.08	1031.01
smooth setting	95.43	382.17	9.64	0.41	812.24

**Table 2:** AFSL results for the rough and smooth high-dimensional simulation setting. Prediction error, computation time and number of correctly and wrongly identified predictors are presented. This results have to be compared with Figure 3 and 4 for the estimation and with Table 1 for the computational efficiency.

## 5.2 Comparison with previous methods

### 5.2.1 The high dimensional setting

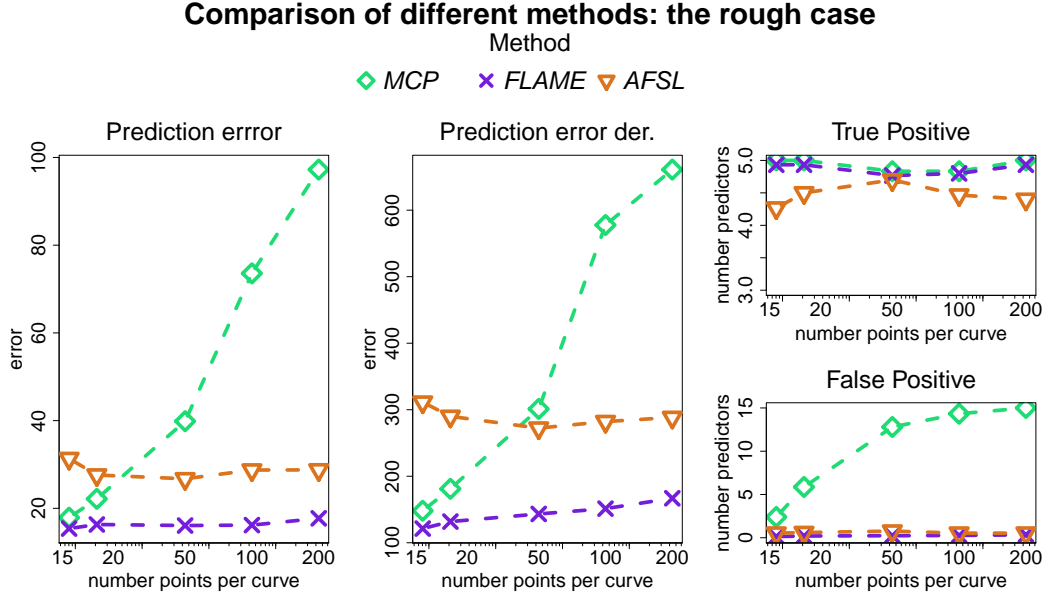
In this section we apply AFLS to the simulation setting we’ve introduced in Section 5.1 and in Table 2 we present the results of AFSL estimation in terms of prediction error, computation time and number of predictors identified (True Positive and False Positive).

A great advantage of FLAME is the reduction of the computation time: FLAME takes much less than AFSL to run and it also achieves better statistical performance. Mainly in the rough case, the Exponential and the Sobolev kernel (with  $\sigma > 1$ ) perform better in terms of prediction error on data, derivatives and in the number of true positive and false positive predictors.

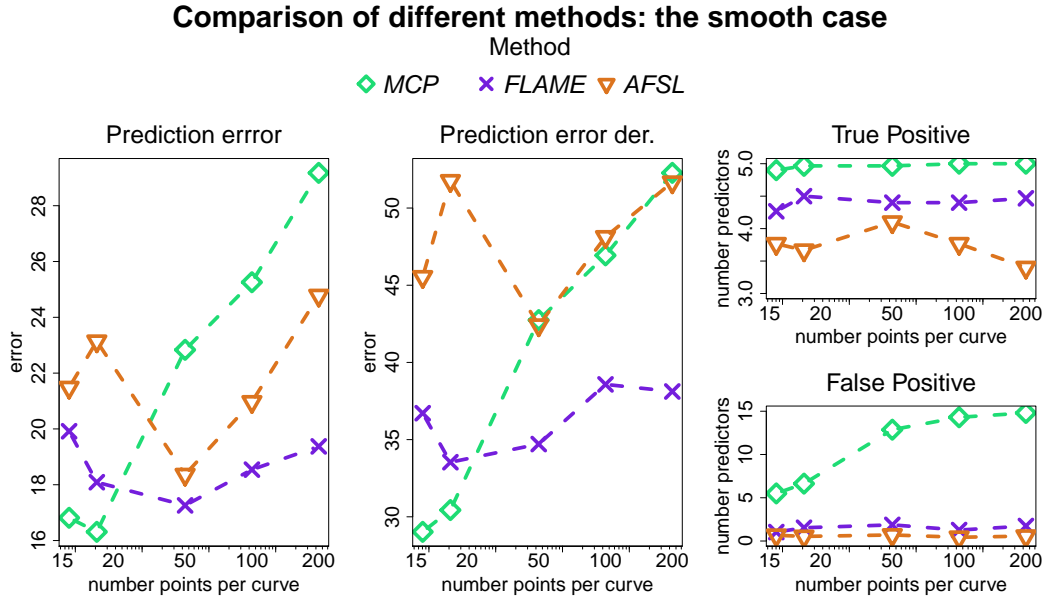
### 5.2.2 The small dimensional setting

In this section we reduce the simulation size to make the application of MCP possible; this method is suitable just for  $N > I$  schemes. We present the results of FLAME, MCP, and AFSL with the same rough and smooth settings introduced in Section 5.1, but with  $N = 50$ ,  $I = 20$  and  $I_0 = 5$ . Moreover we focus on the number of points per curve  $m$  to detect whether these three methods are affected by  $m$ . For FLAME we focus on the Sobolev kernel with  $\sigma = 8$ , since, from Section 5.1, it is shown to be a suitable kernel for both these two settings.

In Figure 5 and 6 the results for the three methods varying  $m$  are shown. We notice that both FLAME and AFSL estimations are almost invariant with respect to  $m$ , while MCP is



**Figure 5:** Summary of the simulations varying the method for the rough case. From the left, the prediction error, the prediction error on derivatives, and the number of true and false positive predictors.



**Figure 6:** Summary of the simulations varying the method for the smooth case. From the left, the prediction error, the prediction error on derivatives, and the number of true and false positive predictors.

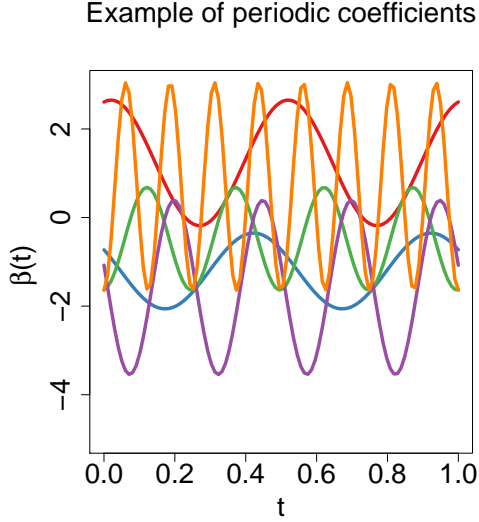
$m$	MCP	FLAME	AFSL	$m$	MCP	FLAME	AFSL
15	36.00	12.90	7.34	15	12.84	76.85	7.75
20	32.20	12.56	7.20	20	13.89	60.39	6.92
50	92.35	13.00	7.28	50	66.30	45.106	8.11
100	126.58	12.08	7.15	100	139.86	92.57	7.00
200	377.36	13.95	6.54	200	221.36	85.45	6.14

**Table 3:** Median time (sec.) for the simulations varying method for the rough (left panel) and smooth case (right panel) in the small dimensional setting.

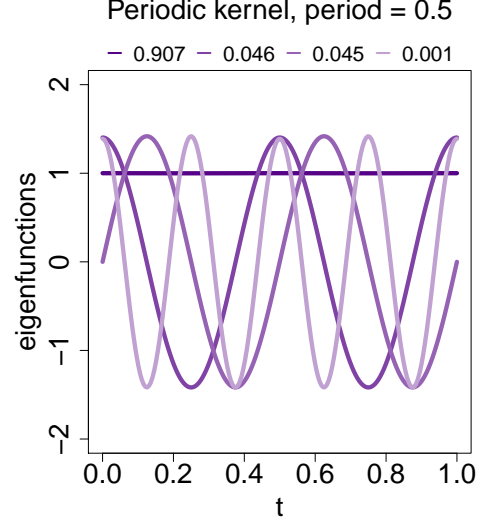
strongly affected by variations of  $m$ , becoming very unreliable when the number of points per curve is large. However, if the number of points is small, MCP performs better than FLAME and AFSL in terms of prediction error and selecting true predictors, mainly in the smooth setting, but still often has trouble in terms of false positives. Focusing on the computational efficiency, presented in Table 3 we notice that FLAME and AFSL are comparable, with the well known higher efficiency of FLAME in the rough case with respect to the smooth, and they both are almost invariant with the change of  $m$ . They globally perform significantly better than MCP, which in addition becomes slower and slower with the increase of  $m$ . The difference in the efficiency of FLAME and AFSL is due to the method used to solve the problem: the coordinate descent method of FLAME is faster than ADMM of AFSL in the high dimensional setting since it is not based on matrix algebra operations, while in the small setting both coordinate descent and ADMM are efficient.

### 5.2.3 The periodic setting

In this section we focus on a distinctive feature of FLAME: the possibility of adapting the choice of the kernel to the prior knowledge on the data. For example in Figure 7 we plot several periodic coefficients  $\beta^*$ . When using FLAME with a periodic kernel, the resulting estimates will also be periodic. In Figure 8, for example, the eigenfunctions of the periodic kernel with period  $1/2$  are shown. This kernel is general enough to be used for the estimations in a simulation setting where  $\beta^*$  functions are sampled as periodic functions with period varying in  $\{1/2, 1/4, 1/8\}$ . AFSL and MCP, on the contrary, don't allow this



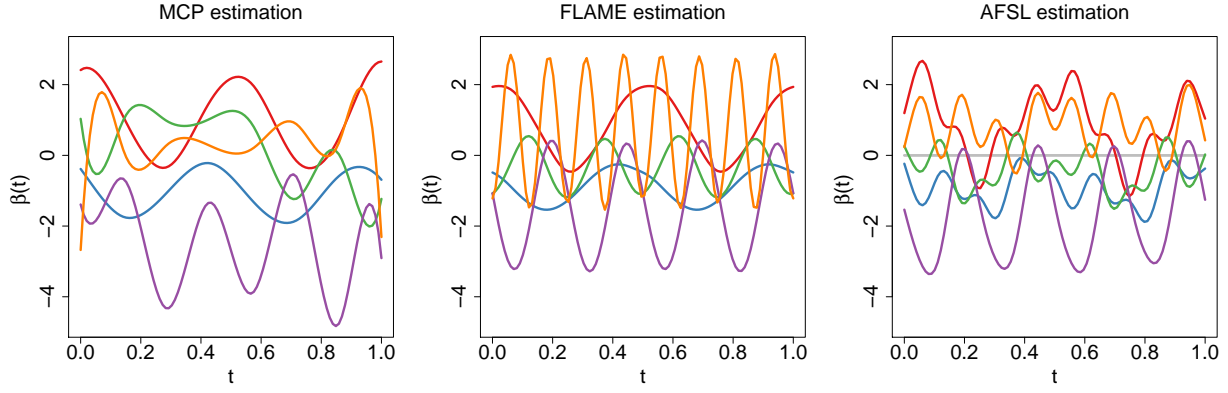
**Figure 7:** Example of 5  $\beta^*$  periodic coefficients, two have period 0.5, two 0.25 and one 0.125.



**Figure 8:** First four eigenfunctions of the periodic kernel with period 0.5. Correspondent explained variability is shown in the top legend

characterizations of the coefficients.

The design matrix  $\mathbf{X}$  is the standardized realization of a multivariate normal distribution with 0 average and identity covariance structure and the errors are sampled from a Matérn process with parameter  $(\nu = 1.5, \text{range} = 1/4, \sigma^2 = 1)$ . The aim is to compare the results of FLAME, MCP, and AFSL. In this particular case, a kernel with period  $\{1/2\}$  allows FLAME to estimate all the predictors identifying also their periodicity. MCP and AFSL, in contrast, are estimated in the general  $L^2$  space, without any further specifications. In Table 4 we present a summary of the average results across 100 replications for the three methods; where we see a fairly dramatic increase in statistical performance for FLAME. An example of the estimates produced by the different methods, based on  $\beta^*$  from Figure 7, is given in Figure 9, where we see again a fairly dramatic advantage when using FLAME.



**Figure 9:** Example of the estimation of the functions of Figure 7 with, from the left, FLAME, MCP and AFSL.

	prediction error	prediction error der.	True Positive	False Positive	Time
FLAME	24.99	666.15	4.93	0.03	25.99
MCP	162.24	4055.37	5	5	924.98
AFSL	54.54	2081.90	4.87	0.53	8.04

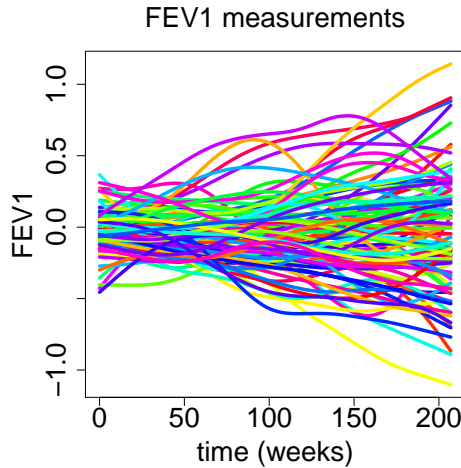
**Table 4:** Comparison of the results of the three methods on simulations in the periodic setting. Average prediction error on data, derivatives, average number of true positive, false positive and the median computational time are shown.

### 5.3 Childhood Asthma Management Program

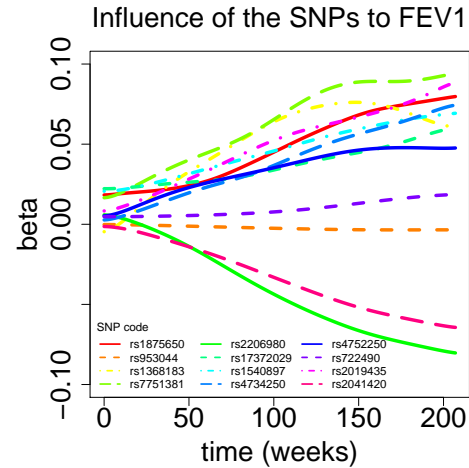
In this section we present the application of FLAME to a large genetic dataset collected from The Childhood Asthma Management Program Research Group (1999). The Childhood Asthma Management Project, CAMP, is a longitudinal trial to analyze the longterm impacts of several daily treatments on children with asthma. It includes 439 Caucasian children, ages 5-12, affected by asthma and monitored for 4 years. These data are freely available from the dbGaP, Study Accession phs000166.v2.p1 (dbGaP (2009)).

Genotypic informations consists of approximately 670,000 SNPs with minor allele frequency larger than 5%. We first apply a screening tool from Chu et al. (2016) to isolate a subset of  $I = 10,000$  SNPs, on which we apply FLAME. The focus of our analysis is, then, the detection of the significant SNPs among these 10,000.

Each child is given one of three treatments: Budesonide, Nedocromil, or a placebo. We account for age at the beginning of the study and gender. To quantify the lung strength



**Figure 10:** FEV1 curves of 100 randomly selected children measured on 4 years of follow up. The contribution of age, gender and treatment have already been removed.



**Figure 11:** Coefficients of the influent SNPs detected and estimated by FLAME.

of children we consider 16 longitudinal measurements of the Forced Expiratory Volume in one second (FEV1), a common proxy for lung strength. The lung capacity is the response function of our linear model and we convert it into a functional data object with a cubic B-spline basis projection with penalty on the second derivative and smoothing parameter chosen via generalized cross-validation.

As a first preprocessing step we remove the influence of gender, age, and treatment from FEV1 and then we apply FLAME to evaluate the impact of the SNPs to the residual functions shown in Figure 10. In Figure 11 the FLAME estimation is presented; for this analysis we use the Sobolev kernel with  $\sigma = 8$ , a 200 points grid for  $\lambda$  with the ratio  $r_\lambda = 0.01$ . We identify the presence of 12 significant SNPs, 9 with a positive effect in the lung development and 3 (rs2206980, rs2041420 and rs953044) with a negative contribution. In Table 5 the list of the identified SNPs with the comparison with the ones identified by AFSL: we notice that FLAME identifies two more SNPs, one with positive effect (rs722490) and one with negative effect (rs2041420).

To add a further comparison with AFSL we identify a test (80% of data) and a training

SNP		AFSL	FLAME
chr	name		
1	rs1875650	+	+
2	rs953044	-	-
5	rs1368183	+	+
6	rs7751381	+	+
6	rs2206980	-	-
7	rs17372029	+	+
8	rs1540897	+	+
8	rs4734250	+	+
10	rs4752250	+	+
11	rs722490		+
15	rs2019435	+	+
20	rs2041420		-

**Table 5:** List of the identified SNPs with AFSL and FLAME. + identifies the SNPs with positive effect and - the SNPs with negative effect, empty cells identify non detected SNPs. Informations on the chromosome location of SNPs and further details can be found in the ALFRED database (Rajeevan et al. (1999)).

set to compute the prediction error of data as  $\sum_{n=1}^N \|Y_n - \mathbf{X}_n \hat{\beta}\|_{L^2}$ . We replicate this analysis 10 times to present a robust conclusion. The average prediction error for FLAME is 0.200, while for AFSL is 0.205. Moreover measuring the computational time we have for FLAME a median of 172.01 sec. and for AFSL 365.07 sec. showing the great advantage of FLAME in terms of computational time, with also a little improvement in term of prediction error.

As a last point, the SNP selected by FLAME but not by AFSL, rs2041420, is located on the gene MACROD2. This gene has been associated with a number of negative health outcomes including Autism, Celiac disease, Crohn’s disease, and Parkinson’s disease (<http://www.gwascentral.org>). It has also been linked to FEV1 and lung development (Strachan et al., 2007; Repapi et al., 2010). However, neither of these previous studies were based on CAMP, and therefore helps validate this finding.

## References

Barber, R., Reimherr, M. and Schill, T. (2016) The function-on-scalar lasso with applications to longitudinal GWAS. *arXiv preprint arXiv:1610.07403*.

- Barbu, V. and Precupanu, T. (2012) *Convexity and optimization in Banach spaces*. Springer Science & Business Media.
- Bauschke, H. H. and Combettes, P. L. (2011) *Convex analysis and monotone operator theory in Hilbert spaces*. Springer Science & Business Media.
- Berlinet, A. and Thomas-Agnan, C. (2011) *Reproducing kernel Hilbert spaces in probability and statistics*. Springer Science & Business Media.
- Boyd, S. and Vandenberghe, L. (2004) *Convex optimization*. Cambridge university press.
- Bühlmann, P., Kalisch, M. and Maathuis, M. (2010) Variable selection in high-dimensional linear models: partially faithful distributions and the pc-simple algorithm. *Biometrika*, **97**, 261–278.
- Cardot, H., Mas, A. and Sarda, P. (2007) Clt in functional linear regression models. *Probability Theory and Related Fields*, **138**, 325–361.
- Chen, Y., Goldsmith, J. and Ogden, T. (2016) Variable selection in function-on-scalar regression. *Stat.*
- Chu, W., Li, R. and Reimherr, M. (2016) Feature screening for time-varying coefficient models with ultrahigh-dimensional longitudinal data. *Ann. Appl. Stat.*, **10**, 596–617. URL: <http://dx.doi.org/10.1214/16-AOAS912>.
- dbGaP (2009) SHARP - national heart, lung, and blood institute snp health association asthma resource project. [http://www.ncbi.nlm.nih.gov/projects/gap/cgi-bin/study.cgi?study\\_id=phs000166.v2.p1](http://www.ncbi.nlm.nih.gov/projects/gap/cgi-bin/study.cgi?study_id=phs000166.v2.p1).
- Dunford, N. and Schwartz, J. (1963) *Linear operators. Part 2: Spectral theory. Self adjoint operators in Hilbert space*. Interscience Publishers.
- Fan, J. and Reimherr, M. (2016) Adaptive function-on-scalar regression. *arXiv preprint arXiv:1610.07507*.
- Fan, Y., James, G. and Radchenko, P. (2015) Functional Additive Regression. *Annals of Statistics*, **43**, 2296–2325.
- Gertheiss, J., Maity, A. and Staicu, A. (2013) Variable selection in generalized functional linear models. *Stat*, **2**, 86–101.
- Graves, S., Hooker, G. and Ramsay, J. (2009) *Functional Data Analysis with R and MATLAB*. Springer.
- Hastie, T., Tibshirani, R. and Friedman, J. (2001) *Elements of Statistical Learning*. Springer.
- Hastie, T., Tibshirani, R. and Wainwright, M. (2015) *Statistical learning with sparsity: the lasso and generalizations*. CRC Press.
- Horváth, L. and Kokoszka, P. S. (2012) *Inference for Functional Data with Applications*. Springer.
- Hsing, T. and Eubank, R. (2015) *Theoretical Foundations of Functional Data Analysis, with an Introduction to Linear Operators*. John Wiley & Sons.

- Huang, J., Ma, S. and Zhang, C.-H. (2008) Adaptive lasso for sparse high-dimensional regression models. *Statistica Sinica*, 1603–1618.
- James, G., Hastie, T., Witten, D. and Tibshirani, R. (2013) *An Introduction to Statistical Learning: With Applications in R*. Springer Texts in Statistics. Springer London, Limited. URL: <http://books.google.com/books?id=at1bmAEACAAJ>.
- Kokoszka, P. and Reimherr, M. (2017) *Introduction to Functional Data Analysis*. Chapman & Hall.
- Laha, R. and Rohatgi, V. (1979) *Probability Theory*. Wiley, New York.
- Lian, H. (2013) Shrinkage estimation and selection for multiple functional regression. *Statistica Sinica*, **23**, 51–74.
- Matsui, H. and Konishi, S. (2011) Variable selection for functional regression models via the L1 regularization. *Computational Statistics & Data Analysis*, **55**, 3304–3310.
- Rajeevan, H., Soundararajan, U., Stein, S., Kidd, K. K. and Miller, P. (1999) ALFRED - the allele frequency database. <https://alfred.med.yale.edu/alfred/AboutALFRED.asp>. Yale University.
- Ramsay, J. O. and Silverman, B. (2006) *Functional data analysis*. Wiley Online Library.
- Repapi, E., Sayers, I., Wain, L. V., Burton, P. R., Johnson, T., Obeidat, M., Zhao, J. H., Ramasamy, A., Zhai, G., Vitart, V. et al. (2010) Genome-wide association study identifies five loci associated with lung function. *Nature genetics*, **42**, 36–44.
- Shor, N. Z. (2012) *Minimization methods for non-differentiable functions*, vol. 3. Springer Science & Business Media.
- Sriperumbudur, B. and Szabó, Z. (2015) Optimal rates for random fourier features. In *Advances in Neural Information Processing Systems*, 1144–1152.
- Strachan, D. P., Rudnicka, A. R., Power, C., Shepherd, P., Fuller, E., Davis, A., Gibb, I., Kumari, M., Rumley, A., Macfarlane, G. J. et al. (2007) Lifecourse influences on health among british adults: effects of region of residence in childhood and adulthood. *International journal of epidemiology*, **36**, 522–531.
- The Childhood Asthma Management Program Research Group (1999) The childhood asthma management program (CAMP): design, rationale, and methods. *Controlled Clinical Trials*, **20**, 91–120.
- Zhang, C.-H. (2010) Nearly unbiased variable selection under minimax concave penalty. *The Annals of statistics*, 894–942.
- Zhao, P. and Yu, B. (2006) On model selection consistency of lasso. *Journal of Machine Learning Research*, **7**, 2541–2563.

# Online Supplemental Material

## A Subgradient Equations for FLAME

Before deriving (1) we state the following Lemma which can found in any of the discussed references on convex analysis.

**Lemma 1** *Let  $f_1 : \mathbb{H} \rightarrow \mathbb{R}$  be  $f_2 : \mathbb{H} \rightarrow \mathbb{R}$  be two convex functionals over a real separable Hilbert space  $\mathbb{H}$ . Then we have the following.*

1. *If the Fréchet derivative of  $f_1$  exists at a point  $x \in \mathbb{H}$ , then the subdifferential of  $f_1$  at  $x$  consists of single point which is the derivative of  $f_1$  at  $x$ .*
2. *The subdifferential of  $f_1 + f_2$  is the sum of their respective subdifferentials:  $\partial(f_1 + f_2) = \partial f_1 + \partial f_2$ . Where the sum is understood as Minkowski sum between two sets.*

We now state two lemmas from Fan and Reimherr (2016)

**Lemma 2** 1. *Consider the functional  $f(x) = \|x\|_{\mathbb{H}}^2$ . Then  $f$  is convex and everywhere differentiable with*

$$\partial f(x) = 2x.$$

2. *Consider the functional  $f(x) = \|x\|_{\mathbb{H}}$ . Then  $f$  is convex and differentiable when  $x \neq 0$  in which case*

$$\partial f(x) = \|x\|_{\mathbb{H}}^{-1}x \quad x \neq 0.$$

*When  $x = 0$  we have*

$$\partial f(0) = \{x \in \mathbb{H} : \|x\| \leq 1\}.$$

We now derive the FLAME subgradient equations. First, we rewrite them using a common norm:

$$L_{\lambda}(\beta) = \frac{1}{2N} \|K^{1/2}(Y - \mathbf{X}\beta)\|_{\mathbb{K}}^2 + \lambda \sum_{i=1}^I \tilde{\omega}_i \|\beta_i\|_{\mathbb{K}}.$$

So  $L_{\lambda}$  is a convex function from  $\mathbb{K}^I \rightarrow \mathbb{R}$ . Here it is also understood that  $K^{1/2}(Y)$  is applied coordinate wise to each function. Since  $\mathbb{K}$  is a real separable Hilbert space we have by Lemma 2.1 and the chain rule that

$$\frac{\partial}{\partial \beta_i} \frac{1}{2N} \|K^{1/2}(Y - \mathbf{X}\beta)\|_{\mathbb{K}}^2 = \frac{1}{N} \sum_{n=1}^N X_{n,i} (K^{1/2}(Y - \mathbf{X}\beta)).$$

By Lemma 2.2 we have that

$$\frac{\partial}{\partial \beta_i} \lambda \sum_{j=1} \tilde{\omega}_j \|\beta_j\|_{\mathbb{K}} = \lambda \tilde{\omega}_j \begin{cases} \|\beta_j\|_{\mathbb{K}}^{-1} \beta_j & \beta_j \neq 0 \\ \{h \in \mathbb{H} : \|h\|_{\mathbb{K}} \leq 1\} & \beta_j = 0 \end{cases}.$$

Applying Lemma 1 we can combine the two subdifferentials to obtain (1).

## B Proofs

The following two lemmas follow from Barber et al. (2016).

**Lemma 3** *If Assumption 2 holds, the FSL estimate  $\tilde{\beta}$ , computed with all the weights set to 1, satisfies*

$$\sup_{i \in \mathcal{S}} \|\beta_i^* - \tilde{\beta}_i\|_{\mathbb{H}} = O_P(r_N^{1/2}) \quad \text{where} \quad r_N = \frac{\log(I)I_0}{N}.$$

**Lemma 4** *Let  $X$  be an  $\mathbb{H}$  valued Gaussian process with mean zero and covariance operator  $C$ . Then we have the bound*

$$P \left\{ \|X\|_{\mathbb{H}}^2 \geq \|C\|_1 + 2\|C\|_2 \sqrt{t} + 2\|C\|_{\infty} t \right\} \leq \exp(-t)$$

where  $\|C\|_1$  the sum of the eigenvalues of  $C$ ,  $\|C\|_2^2$  the sum of the squared eigenvalues and  $\|C\|_{\infty}$  the largest one.

**Corollary 1** *Given the Gaussian process  $X$ , with zero mean and covariance operator  $C$ , and given the kernel operator  $K$  (represented by the eigenvalues  $\theta_j$ :  $\theta_1 \geq \theta_2 \geq \dots \geq 0$ , and the eigenvectors  $v_j$  which define an orthogonal basis for  $\mathbb{H}$  and  $\mathbb{K}$ ), we can prove that*

$$P \left\{ \|K(X)\|_{\mathbb{K}}^2 \geq \theta_1(\|C\|_1 + 2\|C\|_2 \sqrt{t} + 2\|C\|_{\infty} t) \right\} \leq \exp(-t)$$

**PROOF** From the definition of the  $\mathbb{K}$  and  $\mathbb{H}$  norm we obtain that

$$\|K(X)\|_{\mathbb{K}}^2 = \sum_{j=1}^{\infty} \frac{\langle \theta_j X, v_j \rangle^2}{\theta_j} = \sum_{j=1}^{\infty} \theta_j \langle X, v_j \rangle^2 \leq \theta_1 \sum_{j=1}^{\infty} \langle X, v_j \rangle^2 = \theta_1 \|X\|_{\mathbb{H}}^2$$

Then, since from Lemma 4 we have that

$$P(\|X\|_{\mathbb{H}} < f(C, t)) \geq 1 - \exp(-t)$$

with  $f(C, t) = \|C\|_1 + 2\|C\|_2 \sqrt{t} + 2\|C\|_{\infty} t$ .

we prove the statement

$$P(\|K(X)\|_{\mathbb{K}} < \theta_1 f(C, t)) \geq 1 - \exp(-t) \Rightarrow P(\|K(X)\|_{\mathbb{K}} \geq \theta_1 f(C, t)) \leq \exp(-t)$$

■

## Proof of Theorem 1.1

We begin by partitioning the set of the estimated parameters into  $\hat{\mathcal{S}}$  and  $\hat{\mathcal{S}}^C$  where

$$\hat{\mathcal{S}} = \left\{ i \in \{1, \dots, I\} : \hat{\beta}_i \neq 0 \right\}.$$

Our aim for this section is then to prove that, with high probability,  $\mathcal{S} = \hat{\mathcal{S}}$ , that is  $\hat{\beta}$  has  $\mathcal{S}$  as support.

Suppose, for the moment, that  $\hat{\mathcal{S}} = \mathcal{S}$ , then from the subgradient equation (1) we have that

$$(5) \quad \mathbf{X}_1^\top K(Y - \mathbf{X}_1 \hat{\beta}_1) = \lambda \tilde{s}_1 \quad \text{where} \quad \tilde{s}_1 = \left\{ N \tilde{\omega}_i \hat{\beta}_i \|\hat{\beta}_i\|_{\mathbb{K}}^{-1} : i \in \mathcal{S} \right\},$$

and  $\hat{\beta}_1 = \{\hat{\beta}_i : i \in \mathcal{S}\}$  is the estimate of the non-zero predictors. This then implies that

$$K(\hat{\beta}_1) = (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} (\mathbf{X}_1^\top K(Y) - \lambda \tilde{s}_1) = K(\beta_1^*) + (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} (\mathbf{X}_1^\top K(\varepsilon) - \lambda \tilde{s}_1).$$

To prove that  $\beta^*$  and  $\hat{\beta}$  have the same support ( $\mathcal{S} = \hat{\mathcal{S}}$ ) we have to verify the following.

- If  $i \in \mathcal{S}$ ,  $\hat{\beta}_1 \stackrel{\mathbb{S}}{=} \beta_1^*$ , i.e. the true non-zero predictors are correctly identified. This condition can be also written as

$$(6) \quad \|K(\beta_i^*) - K(\hat{\beta}_i)\|_{\mathbb{K}} < \|K(\beta_i^*)\|_{\mathbb{K}}.$$

- If  $i \notin \mathcal{S}$ ,  $\hat{\beta}_i$  is set to zero, so that the zero predictors are correctly detected. That means

$$(7) \quad \left\| \frac{1}{N} \mathbf{X}_i^\top K(Y - \mathbf{X}_1 \hat{\beta}_1) \right\|_{\mathbb{K}} < \lambda \tilde{\omega}_i$$

To achieve a better definition of (6) and (7) we introduce the definition of  $Y$  and find, for

all  $i \in \mathcal{S}$

$$\|K(\beta_i^*) - K(\hat{\beta}_i)\|_{\mathbb{K}} < \|K(\beta_i^*)\|_{\mathbb{K}} \implies \left\| e_i^\top \left[ N^{-1} \hat{\Sigma}_{11}^{-1} (\mathbf{X}_1^\top K(\varepsilon) - \lambda \tilde{s}_1) \right] \right\|_{\mathbb{K}} < \|K(\beta_i^*)\|_{\mathbb{K}}$$

with  $e_i$  a  $I$ -size vector with all zero coefficient but the  $i^{th}$  which is 1 and  $\hat{\Sigma}_{11}$  the estimated covariance matrix of  $\mathbf{X}_1$ :  $\hat{\Sigma}_{11} = N^{-1} \mathbf{X}_1^\top \mathbf{X}_1$ . While, for all  $i \notin \mathcal{S}$

$$\left\| \frac{1}{N} \mathbf{X}_i^\top K(Y - \mathbf{X}_1 \hat{\beta}_1) \right\|_{\mathbb{K}} < \lambda \tilde{\omega}_i \implies \left\| \mathbf{X}_i^\top N^{-1} [H K(\varepsilon) + \lambda \mathbf{X}_1 (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \tilde{s}_1] \right\|_{\mathbb{K}} < \lambda \tilde{\omega}_i$$

with  $H = (I - \mathbf{X}_1 (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top)$ .

Considering the event  $\{\mathcal{S} = \hat{\mathcal{S}}\}$ , we observe that

$$\{\mathcal{S} \neq \hat{\mathcal{S}}\} \subset B_1 \cup B_2 \cup B_3 \cup B_4$$

with

$$\begin{aligned} B_1 &= \left\{ \frac{1}{N} \|e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top K(\varepsilon)\|_{\mathbb{K}} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}}{2} : \text{for some } i \in \mathcal{S} \right\} \\ B_2 &= \left\{ \frac{\lambda}{N} \|e_i^\top \hat{\Sigma}_{11}^{-1} \tilde{s}_1\|_{\mathbb{K}} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}}{2} : \text{for some } i \in \mathcal{S} \right\} \\ B_3 &= \left\{ \frac{1}{N} \|\mathbf{X}_i^\top H K(\varepsilon)\|_{\mathbb{K}} \geq \frac{\lambda \tilde{\omega}_i}{2} : \text{for some } i \notin \mathcal{S} \right\} \\ B_4 &= \left\{ \frac{1}{N^2} \|\mathbf{X}_i^\top \mathbf{X}_1 \hat{\Sigma}_{11}^{-1} \tilde{s}_1\|_{\mathbb{K}} \geq \frac{\tilde{\omega}_i}{2} : \text{for some } i \notin \mathcal{S} \right\}. \end{aligned}$$

We will show that with  $N$  increasing  $P(B_l) \rightarrow 0$  for  $l = 1, \dots, 4$  and then  $P(\hat{\mathcal{S}} \neq \mathcal{S}) \rightarrow 0$ .

**Step 1:**  $P(B_1) \rightarrow 0$

Given

$$B_1 = \left\{ \frac{1}{N} \|e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top K(\varepsilon)\|_{\mathbb{K}} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}}{2} : \text{for some } i \in \mathcal{S} \right\}$$

we notice that  $B_1 = \cup_{i \in \mathcal{S}} A_i$  where

$$A_i = \left\{ \frac{1}{N} \|e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top K(\varepsilon)\|_{\mathbb{K}} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}}{2} \right\} = \left\{ \frac{1}{N^2} \|e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top K(\varepsilon)\|_{\mathbb{K}}^2 \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}^2}{4} \right\}$$

and we have that  $P(B_1) \leq \sum_{i \in \mathcal{S}} P(A_i)$ . For each  $i$  we have that

$$\frac{1}{N^2} \|e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top K(\varepsilon)\|_{\mathbb{K}}^2 = \|K(T_i)\|_{\mathbb{K}}^2$$

where  $T_i = N^{-1}e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top \varepsilon$  is a Gaussian process (in  $\mathbb{H}$ ) with zero mean and covariance operator  $C_T$

$$\begin{aligned} C_T &= N^{-1}e_i^\top \hat{\Sigma}_{11}^{-1} \mathbf{X}_1^\top \mathbf{X}_1 \left( \hat{\Sigma}_{11}^{-1} \right)^\top e_i N^{-1}C \\ &= N^{-1}e_i^\top \hat{\Sigma}_{11}^{-1} N \hat{\Sigma}_{11} \hat{\Sigma}_{11}^{-1} e_i N^{-1}C = N^{-1}e_i^\top \hat{\Sigma}_{11}^{-1} e_i C. \end{aligned}$$

Recall  $C$  the covariance operator of the error process  $\varepsilon$ . From Corollary 1 we have that

$$P \left\{ \|K(T_i)\|_{\mathbb{K}}^2 \geq \theta_1 N^{-1} e_i^\top \hat{\Sigma}_{11}^{-1} e_i (\|C\|_1 + 2\|C\|_2 \sqrt{t} + 2\|C\|_\infty t) \right\} \leq \exp(-t).$$

Define  $\tilde{t}$  such that

$$\frac{\|K(\beta_i^*)\|_{\mathbb{K}}^2}{4} \geq \theta_1 N^{-1} e_i^\top \hat{\Sigma}_{11}^{-1} e_i \left( \|C\|_1 + 2\|C\|_2 \sqrt{\tilde{t}} + 2\|C\|_\infty \tilde{t} \right)$$

so then

$$\begin{aligned} P(A_i) &= P \left( \|K(T_i)\|_{\mathbb{K}} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}}{2} \right) \\ &\leq P \left( \|K(T_i)\|_{\mathbb{K}}^2 \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}^2}{4} \right) \\ &\leq P \left( \|K(T_i)\|_{\mathbb{K}}^2 \geq \theta_1 N^{-1} e_i^\top \hat{\Sigma}_{11}^{-1} e_i \left( \|C\|_1 + 2\|C\|_2 \sqrt{\tilde{t}} + 2\|C\|_\infty \tilde{t} \right) \right) \\ &\leq \exp(-\tilde{t}) \end{aligned}$$

We can define a constant  $c$  such that

$$\left( \|C\|_1 + 2\|C\|_2 \sqrt{t} + 2\|C\|_\infty t \right) \leq ct$$

so that  $\tilde{t}$  can satisfy the simpler inequality

$$\frac{\|K(\beta_i^*)\|_{\mathbb{K}}^2}{4} \geq \frac{1}{N} \theta_1 e_i^\top \hat{\Sigma}_{11}^{-1} e_i c \tilde{t}.$$

Recall  $b_N = \min_{i \in \mathcal{S}} \|K(\beta_i^*)\|_{\mathbb{K}}$ , so then

$$\frac{b_N^2}{4} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}^2}{4} \geq \frac{1}{N} \theta_1 e_i^\top \hat{\Sigma}_{11}^{-1} e_i c \tilde{t}.$$

From Assumption 2.3

$$e_i^\top \hat{\Sigma}_{11}^{-1} e_i \leq \nu_1$$

then  $\tilde{t}$  s.t.

$$\tilde{t} \leq \frac{Nb_N^2}{4\theta_1\nu_1c}$$

and so, taking  $t$  equal to the upper bound we have that

$$P(A_i) \leq \exp\left(-\frac{Nb_N^2}{4\theta_1\nu_1c}\right)$$

And, coming back to the statement on  $B_1$ , we can apply Assumption 2.1 to conclude that

$$P(B_1) \leq \sum_{i \in \mathcal{S}} P(A_i) \leq I_0 \exp\left(-\frac{Nb_N^2}{4\nu_1\theta_1c}\right) = \exp\left(-\frac{Nb_N^2}{4\theta_1\nu_1c} + \log(I_0)\right) \rightarrow 0.$$

**Step 2:**  $P(B_2) \rightarrow 0$

Recall that

$$B_2 = \left\{ \frac{\lambda}{N} \|e_i^\top \hat{\Sigma}_{11}^{-1} \tilde{s}_1\|_{\mathbb{K}} \geq \frac{\|K(\beta_i^*)\|_{\mathbb{K}}}{2} : \text{ for some } i \in \mathcal{S} \right\}$$

with  $\tilde{s}_1 = \left\{ N\tilde{\omega}_i \hat{\beta}_i \|\hat{\beta}_i\|_{\mathbb{K}}^{-1} \mid i \in \mathcal{S} \right\}$ . The  $\mathbb{K}$  norm of  $\tilde{s}_1$  is given by

$$\|\tilde{s}_1\|_{\mathbb{K}}^2 = \sum_{i \in \mathcal{S}} N^2 \tilde{\omega}_i^2 \frac{\|\hat{\beta}_i\|_{\mathbb{K}}^2}{\|\hat{\beta}_i\|_{\mathbb{K}}^2} = N^2 \sum_{i \in \mathcal{S}} \tilde{\omega}_i^2 = N^2 \left( \sum_{i \in \mathcal{S}} \omega_i^2 + \sum_{i \in \mathcal{S}} (\tilde{\omega}_i^2 - \omega_i^2) \right),$$

where  $\tilde{\omega}_i = \|\tilde{\beta}_i\|_{\mathbb{H}}^{-1}$  is computed using FSL and  $\omega_i = \|\beta_i^*\|_{\mathbb{H}}^{-1}$ . Since the  $\tilde{\beta}_i$  are consistent in  $\mathbb{H}$  (uniformly in  $i$ ) we can apply the reverse triangle inequality several times to arrive at

$$|\tilde{\omega}_i^2 - \omega_i^2| \leq \frac{\|\beta_i^* - \tilde{\beta}_i\|_{\mathbb{H}}}{\|\beta_i^*\|_{\mathbb{H}}^3} (2 + o_P(1)),$$

where the  $o_P(1)$  again holds uniformly across  $i \in \mathcal{S}$ . From the definition of  $b_N = \min_{i \in \mathcal{S}} \|K(\beta_i^*)\|_{\mathbb{K}}$  we have that for all  $i \in \mathcal{S}$

$$b_N \leq \|K(\beta_i^*)\|_{\mathbb{K}} \leq \theta_1^{1/2} \|\beta_i^*\|_{\mathbb{H}}$$

and moreover from the definition of the rate  $r_N$  of Lemma (3), uniformly in  $i$

$$\|\beta_i^* - \tilde{\beta}_i\|_{\mathbb{H}} \leq \sup_{i \in \mathcal{S}} \|\beta_i^* - \tilde{\beta}_i\|_{\mathbb{H}} = O_P(r_N^{1/2}).$$

Then, uniformly in  $i \in \mathcal{S}$

$$|\tilde{\omega}_i^2 - \omega_i^2| \leq \frac{2}{\|\beta_i^*\|_{\mathbb{H}}^2} \frac{\theta_1^{1/2}}{b_N} \|\beta_i^* - \tilde{\beta}_i\|_{\mathbb{H}} \leq \frac{\theta_1^{1/2}}{b_N} O_P(r_N^{1/2}) \omega_i^2.$$

By Assumption 2,  $r_N^{1/2}/b_N \rightarrow 0$ , and so we conclude

$$\begin{aligned}
\|\tilde{s}_1\|_{\mathbb{K}}^2 &\leq N^2 \left( \sum_{i \in \mathcal{S}} \omega_i^2 \right) (1 + o_p(1)) = N^2 \left( \sum_{i \in \mathcal{S}} \frac{1}{\|\beta_i^*\|_{\mathbb{H}}^2} \right) (1 + o_p(1)) \\
(8) \quad &\leq N^2 \frac{I_0 \theta_1^2}{b_N^2} (1 + o_p(1)).
\end{aligned}$$

Then for the original object we have for each  $i \in \mathcal{S}$

$$\frac{\lambda}{N} \frac{\|e_i^\top \hat{\Sigma}_{11}^{-1} \tilde{s}_1\|_{\mathbb{K}}}{\|K(\beta_i^*)\|_{\mathbb{K}}} \leq \frac{\lambda}{N} \frac{\|e_i^\top \hat{\Sigma}_{11}^{-1}\| \|\tilde{s}_1\|_{\mathbb{K}}}{\|K(\beta_i^*)\|_{\mathbb{K}}}$$

with  $\|e_i^\top \hat{\Sigma}_{11}^{-1}\| \leq \|e_i\| \|\hat{\Sigma}_{11}^{-1}\|_{op} \leq \nu_1$  from Assumption 2 and in the end

$$\frac{\lambda}{N} \frac{\|e_i^\top \hat{\Sigma}_{11}^{-1}\| \|\tilde{s}_1\|_{\mathbb{K}}}{\|K(\beta_i^*)\|_{\mathbb{K}}} \leq \frac{\lambda \nu_1 \sqrt{I_0} N}{N b_N b_N} (1 + o_p(1)) \rightarrow 0.$$

### Step 3

From the previous definition of  $B_3$ :

$$B_3 = \left\{ \frac{1}{N} \|\mathbf{X}_i^\top H K(\varepsilon)\|_{\mathbb{K}} \geq \frac{\lambda \tilde{\omega}_i}{2} : \text{ for some } i \notin \mathcal{S} \right\}$$

we define  $A_i$  s.t. for  $i \notin \mathcal{S}$

$$A_i = \left\{ \frac{1}{N} \|\mathbf{X}_i^\top H K(\varepsilon)\|_{\mathbb{K}} \geq \frac{\lambda \tilde{\omega}_i}{2} \right\}$$

and  $B_3 = \cup_{i \notin \mathcal{S}} A_i$ . We can define the gaussian process  $\mathbf{X}_i H \varepsilon$ , which has zero mean and as covariance operator  $\mathbf{X}_i^\top H H^\top \mathbf{X}_i C = \mathbf{X}_i^\top H \mathbf{X}_i C$ , since  $H$  is symmetric and idempotent, with  $C$  the covariance operator of the zero mean gaussian process  $\varepsilon$ . Moreover, since we have that  $\sup_{i \notin \mathcal{S}} \|\tilde{\beta}_i\|_{\mathbb{H}} = O_P(r_N^{1/2})$  we can notice that  $\tilde{\omega}_i \leq 1/\sup_{i \notin \mathcal{S}} (\|\tilde{\beta}_i\|_{\mathbb{H}})$  and then

$$A_i \subseteq \left\{ O_P(r_N^{1/2}) \|\mathbf{X}_i^\top H K(\varepsilon)\|_{\mathbb{K}} \geq \frac{N\lambda}{2} \right\}.$$

Then for any  $\epsilon > 0$  we can find a  $T = T(\epsilon) > 0$  s.t.

$$P(A_i) \leq \frac{\epsilon}{2(I - I_0)} + P \left( \|\mathbf{X}_i^\top H K(\varepsilon)\|_{\mathbb{K}} \geq \frac{N\lambda}{2T r_N^{1/2}} \right).$$

As we discussed before, to apply Corollary 1, we need to detect  $\tilde{t}$  s.t.

$$(9) \quad \mathbf{X}_i^\top H \mathbf{X}_i (\|C\|_1 + 2\|C\|_2 \sqrt{\tilde{t}} + 2\|C\|_\infty \tilde{t}) \leq \left( \frac{N\lambda}{2Tr_N^{1/2}} \right)^2.$$

Focusing on the left side of the inequality we know that

$$\mathbf{X}_i^\top H \mathbf{X}_i (\|C\|_1 + 2\|C\|_2 \sqrt{\tilde{t}} + 2\|C\|_\infty \tilde{t}) \leq N\tilde{t}c.$$

Since  $H$  is a projection matrix we have

$$\mathbf{X}_i H \mathbf{X}_i = \sum_{t=1}^N \left( \sum_{n=1}^N \mathbf{X}_{i,n} H_{n,t} \right)^2 = \sum_{t=1}^N 1 = N,$$

and again there exists a constant  $c$  such that  $\forall t, ct \geq (\|C\|_1 + 2\|C\|_2 \sqrt{\tilde{t}} + 2\|C\|_\infty \tilde{t})$ , so we define  $\tilde{t}$ :

$$\tilde{t}cN \leq \left( \frac{N\lambda}{2Tr_N^{1/2}} \right)^2 \Rightarrow \tilde{t} = \frac{\lambda^2 N}{4T^2 cr_N}.$$

Applying corollary 1 we have

$$P \left( \|\mathbf{X}_i^\top H K(\varepsilon)\|_{\mathbb{K}} \geq \frac{N\lambda}{2Tr_N^{1/2}} \right) \leq \exp \left( -\frac{\lambda^2 N}{4T^2 cr_N} \right) \leq \exp \left( -\frac{I_0 \log^2(I)}{N4T^2 cr_N} \right)$$

and then we can compute the probability of  $B_3$

$$\begin{aligned} P(B_3) &\leq \sum_{i \notin \mathcal{S}} P(A_i) \leq (I - I_0) \exp \left( -\frac{I_0 \log^2(I)}{4NT^2 cr_N} \right) + \frac{\epsilon}{2} \\ &\leq \exp \left( -\frac{I_0 \log^2(I)}{4NT^2 cr_N} + \log(I - I_0) \right) + \frac{\epsilon}{2}. \end{aligned}$$

Since  $r_N \ll (I_0 \log^2(I))/N$ , we can take  $N$  large enough to make the first term smaller than  $\epsilon/2$  and have the convergence of the probability to 0.

#### Step 4

Recall that  $B_4$  is defined as

$$B_4 = \left\{ \frac{1}{N^2} \|\mathbf{X}_i^\top \mathbf{X}_1 \hat{\Sigma}_{11}^{-1} \tilde{s}_1\|_{\mathbb{K}} \geq \frac{\tilde{\omega}_i}{2} : \text{ for some } i \notin \mathcal{S} \right\}.$$

Recall from (8)

$$\|\tilde{s}_1\|_{\mathbb{K}}^2 \leq N^2 \theta_1^2 \frac{I_0}{b_N^2} (1 + o_p(1)),$$

as well as

$$\sup_{i \notin \mathcal{S}} \tilde{\omega}_i^{-1} = O_P(r_N^{1/2}).$$

The irrerepresentable condition implies

$$\forall i \notin \mathcal{S}, \quad \|\mathbf{X}_i^\top \mathbf{X}_1 \hat{\Sigma}_{11}^{-1}\|_{op} \leq \|\hat{\Sigma}_{21} \hat{\Sigma}_{11}^{-1}\|_{op} \leq \phi < 1.$$

Then we consider the inequality of  $B_4$  for a fixed  $i \notin \mathcal{S}$

$$\frac{2\|\mathbf{X}_i^\top \mathbf{X}_1 \hat{\Sigma}_{11}^{-1} \tilde{s}_1\|_{\mathbb{K}}}{N^2 \tilde{\omega}_i} \leq \frac{2\|\mathbf{X}_i^\top \mathbf{X}_1 \hat{\Sigma}_{11}^{-1}\|_{op} \|\tilde{s}_1\|_{\mathbb{K}}}{N^2 \tilde{\omega}_i} \leq \frac{2\phi r_N^{1/2} I_0^{1/2} \theta_1}{N b_N} O_P(1) \rightarrow 0,$$

which finishes Step 4 and completes the proof.

## Proof of Theorem 1.2

Let  $h_n = \{h_{i,n}\} \in \mathbb{K}^I$  be a bounded sequence:  $\|h_n\|_{\mathbb{K}} < M_1$ . We will show that

$$\frac{\sqrt{N} \langle h_n, \hat{\beta} - \beta^* \rangle_{\mathbb{H}}}{\sigma_n} \xrightarrow{D} \mathcal{N}(0, 1) \quad \text{where} \quad \sigma_n^2 = \sum_{i=1}^{I_0} \sum_{j=1}^{I_0} \hat{\Sigma}_{11;ij}^{-1} \langle h_{i,n}, C h_{j,n} \rangle,$$

assuming that the  $h_{i,n}$  are chosen such that  $\sum_{i \in \mathcal{S}} \langle C^{1/2} h_i, C^{1/2} h_i \rangle \geq M_2 > 0$  for some fixed  $M_2$ . Recall that the oracle estimator is

$$\hat{\beta}_O^{\mathcal{S}} = (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \mathbf{X}_1^\top Y \quad \text{and} \quad \hat{\beta}_O = \{\hat{\beta}_O^{\mathcal{S}}, 0\},$$

where 0 here is the zero function in  $\mathbb{K}^{I-I_0}$ . Since we assume that the  $Y$  are Gaussian, we have that

$$\sqrt{N} \langle h_n, \hat{\beta}_O - \beta_1^* \rangle_{\mathbb{H}} \sim \mathcal{N}(0, \sigma_n^2).$$

By Assumption 2.3 we have that

$$\sigma_n^2 \geq \nu_1^{-1} \sum_{i \in \mathcal{S}} \langle C^{1/2} h_i, C^{1/2} h_i \rangle \geq \nu_1 M_2,$$

and so is bounded from below, so we need only to show that

$$\sqrt{N} \langle h_n, \hat{\beta}_O - \hat{\beta}_1 \rangle_{\mathbb{H}} = o_P(1).$$

From equation 5, when  $\hat{S} = S$  we have that

$$\begin{aligned}\sqrt{N}\langle h, \hat{\beta}_O - \hat{\beta} \rangle_{\mathbb{H}} &= \sqrt{N}\lambda \langle (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} K^{-1}(\tilde{s}_1), h_n^S \rangle_{\mathbb{H}} \\ &= \frac{\lambda}{\sqrt{N}} \langle \Sigma_{11}^{-1} K^{-1/2}(\tilde{s}_1), K^{-1/2} h_n^S \rangle \\ &\leq \frac{\lambda}{\sqrt{N}} \|\Sigma_{11}^{-1} K^{-1/2}(\tilde{s}_1)\|_{\mathbb{H}} \|h_n\|_{\mathbb{K}}.\end{aligned}$$

Applying Assumption 2.3 we have that

$$\frac{\lambda}{\sqrt{N}} \|\Sigma_{11}^{-1} K^{-1/2}(\tilde{s}_1)\|_{\mathbb{H}} \|h_n\|_{\mathbb{K}} \leq \frac{\lambda}{\sqrt{N}\nu_1} \|\tilde{s}_1\|_{\mathbb{K}} \|h_n\|_{\mathbb{K}}.$$

From the equation (8) we have

$$\|\tilde{s}_1\|_{\mathbb{K}} \leq \frac{\sqrt{I_0}N}{b_N} (1 + o_p(1))$$

and then

$$|\sqrt{N}\langle h, \hat{\beta}_O - \hat{\beta}_1 \rangle_{\mathbb{H}}| \leq \frac{\lambda\sqrt{I_0}\sqrt{N}\|h_n\|_{\mathbb{K}}}{\nu_1 b_N} (1 + o_P(1)) = o_P(1),$$

by Assumption 2. Since  $P(\hat{S} = S) \rightarrow 1$  the proof is complete.

## Proof of Theorem 2

We begin by partitioning the problem into two pieces:

$$\begin{aligned}(10) \quad N\|\hat{\beta} - \hat{\beta}_O\|^2 &= N \sum_{i=1}^I \|\hat{\beta}_i - \hat{\beta}_{O,i}\|^2 \\ &= N \sum_{i=1}^I \sum_{j=1}^J \langle \hat{\beta} - \hat{\beta}_O, e_i \otimes v_j \rangle^2 \\ (11) \quad &+ N \sum_{i=1}^I \sum_{j=J+1}^{\infty} \langle \hat{\beta} - \hat{\beta}_O, e_i \otimes v_j \rangle^2.\end{aligned}$$

Bounding (10) follows the similar arguments as in the proof of 1.2, namely

$$\langle \hat{\beta} - \hat{\beta}_O, e_i \otimes v_j \rangle^2 = \frac{\lambda^2}{N^2 \theta_j} \langle \hat{\Sigma}_{11}^{-1} K^{-1/2}(\tilde{s}_1), e_i \otimes v_j \rangle^2 \leq \frac{\lambda^2}{N^2 \theta_j \nu_1^2} \langle K^{-1/2}(\tilde{s}_1), e_i \otimes v_j \rangle^2.$$

This gives the bound

$$N \sum_{i=1}^I \sum_{j=1}^J \langle \hat{\beta} - \hat{\beta}_O, v_j \rangle^2 \leq \frac{\lambda^2}{\theta_J \nu_1^2 N} \|\tilde{s}_1\|_{\mathbb{K}}^2 \leq \frac{\lambda^2 N I_0}{\theta_J \nu_1^2 b_N^2} (1 + o_P(1)).$$

Turning to the second term, we express  $\hat{\beta}$  using a different form. Notice that we can write

$$\tilde{s}_1 = \Lambda \hat{\beta}_1,$$

where  $\Lambda$  is a diagonal matrix of the terms  $\{N \tilde{w}_i \|\hat{\beta}_i\|_K^{-1}\}$ . We therefore have that

$$\mathbf{X}_1^\top K(Y) - (\mathbf{X}_1^\top \mathbf{X}_1) K(\hat{\beta}) - \lambda \Lambda \hat{\beta}_1 = 0$$

We can re-express this equation as

$$\hat{\beta}_O - \hat{\beta}_1 + \lambda (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \Lambda K^{-1}(\hat{\beta}_1) = 0 \implies \hat{\beta}_1 = (I + \lambda (\mathbf{X}_1^\top \mathbf{X}_1)^{-1} \Lambda K^{-1})^{-1} \hat{\beta}_O.$$

The above shrinks (all operators above are positive definite) every coordinate of  $\hat{\beta}_O$  to obtain  $\hat{\beta}_1$  and thus we have that

$$N \sum_{j=J+1}^{\infty} \sum_{i=1}^{\infty} \langle \hat{\beta} - \hat{\beta}_O, e_i \otimes v_j \rangle^2 \leq 4N \sum_{j=J+1}^{\infty} \sum_{i=1}^{\infty} \langle \hat{\beta}_O, e_i \otimes v_j \rangle^2.$$

We compute the expected value

$$\mathbb{E} \langle \hat{\beta}_O, e_i \otimes v_j \rangle^2 = \langle \beta^\star, e_i \otimes v_j \rangle^2 + (\mathbf{X}_1^\top \mathbf{X}_1)_{i,i}^{-1} \langle C v_j, v_j \rangle.$$

This implies that

$$4N \sum_{j=J+1}^{\infty} \sum_{i=1}^{\infty} \langle \hat{\beta}_O, e_i \otimes v_j \rangle^2 = O_P(1) N \left[ \sum_{i=1}^I \sum_{j=J+1}^{\infty} \langle \beta^\star, e_i \otimes v_j \rangle^2 + \sum_{i=1}^I \sum_{j=J+1}^{\infty} (\mathbf{X}_1^\top \mathbf{X}_1)_{i,i}^{-1} \langle C v_j, v_j \rangle \right].$$

Which can be bounded by

$$O_P(1) \left[ N I_0 \theta_J^{1+\delta} B^2 + \frac{I_0}{\nu_1} o(1) \right],$$

as long as  $J \rightarrow \infty$ , since  $C$  is a trace class operator.

To ensure both (10) and (11) go to zero, we require that  $J$  is such that

$$N\theta_J^{1+\delta} \rightarrow 0 \quad \text{and} \quad \frac{\lambda^2 N}{\theta_J b_N^2} \rightarrow 0.$$

So we need to be able to choose  $J$  such that

$$\theta_J \ll N^{-1/(1+\delta)} \quad \text{and} \quad \theta_J \gg \frac{\lambda^2 N}{b_N^2}.$$

This is possible if

$$\frac{\lambda^2 N}{b_N^2} \ll N^{-1/(1+\delta)} \iff \lambda \ll \frac{b_N}{N^{1/2+1/(1+\delta)}},$$

as desired.