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RKHSMetaMod: An R package to estimate the Hoeffding decomposition of an unknown function by solving RKHS ridge group sparse optimization problem

Halaleh Kamari

Université d'Evry Val d'Essonne
and INRA

Sylvie Huet

INRA

Marie-Luce Taupin

Université d'Evry Val d'Essonne

Abstract

In the context of the Gaussian regression model, the package **RKHSMetaMod** allows to estimate a meta model by solving the ridge group sparse optimization problem based on the Reproducing Kernel Hilbert Spaces (RKHS). The obtained estimator is an additive model that satisfies the properties of the Hoeffding decomposition, and its terms estimate the terms in the Hoeffding decomposition of the unknown regression function. The estimators of the Sobol indices are deduced from the estimated meta model. This package provides an interface from R statistical computing environment to the C++ libraries **Eigen** and **GSL**. In order to speed up the execution time, almost all of the functions of the **RKHSMetaMod** package are written using the efficient C++ libraries through **RcppEigen** and **RcppGSL** packages. These functions are then interfaced in the R environment in order to propose an user friendly package.

Keywords: meta model, Hoeffding decomposition, optimization problem, Reproducing Kernel Hilbert Spaces, Sobol indices.

1. Introduction

We consider a Gaussian regression model

$$Y = m(X) + \sigma\varepsilon, \tag{1}$$

where variables $X = \{X_1, \dots, X_d\}$ are distributed independently and identically with a known law $P_X = \prod_{a=1}^d P_{X_a}$ on \mathcal{X} , a compact subset of \mathbb{R}^d . The error ε is distributed as a standard

Normal distribution, i.e. $\varepsilon \sim \mathcal{N}(0, 1)$, and is independent of X . The variance σ^2 is unknown, and the number d of the variables X may be large. The function $m : \mathbb{R}^d \rightarrow \mathbb{R}$ is unknown, it may present high complexity as strong non linearities and high order interaction effects between its coordinates, and we suppose that it is square-integrable, i.e. $m \in L^2(\mathcal{X}, P_X)$.

On the basis of n data points (X_i, Y_i) , $i = 1, \dots, n$, we estimate meta models and perform sensitivity analysis in order to determine the influence of each variable and groups of variables on the output Y . This approach combines the variance-based methods for global sensitivity analysis of complex models and the statistical tools for sparse non-parametric estimation in multivariate Gaussian regression model. The estimated meta model approximates the Hoeffding decomposition of the function m and allows to estimate its Sobol indices. This estimator belongs to a Reproducing Kernel Hilbert Spaces (RKHS) \mathcal{H} , which is constructed as a direct sum of the Hilbert spaces. It is calculated by minimizing a least-squares criteria penalized by the sum of two penalty terms: the Hilbert norm and the empirical norm. Moreover, this procedure allows to select the subsets of variables X that contribute to predict the output Y .

Let us briefly recall the usual context of the global sensitivity analysis, when the function m is known, and the objectives of the meta modelling in this context. Let $g = (g_1, \dots, g_n)$ be the outputs of n runs of the true model m based on n realizations of the input vector X , so $\{X_i\}_{i=1}^n$ is the experimental design and $g_i = m(X_i)$, $i = 1, \dots, n$. A meta model is an approximation of the original model which is built from the experimental design of limited size. In the context of the global sensitivity analysis, the meta model is used in order to quantify the influence of some input variables X or groups of them on the output g . The original model is replaced by the meta model which could be used then to compute the sensitivity indices in negligible time.

Let us introduce some notations. We denote by \mathcal{P} the set of parts of $\{1, \dots, d\}$ with dimensions 1 to d . For all $X \in \mathcal{X}$ and $v \in \mathcal{P}$, X_v represents the vector with components X_a for all $a \in v$. The cardinality of a set A is denoted by $|A|$. For all $v \in \mathcal{P}$, $m_v : \mathbb{R}^{|v|} \rightarrow \mathbb{R}$ denotes a function of X_v .

The independency between the input variables X allows to write the function m according to its Hoeffding decomposition (Hoeffding (1948), Sobol (1993), Van der Vaart (1998)):

$$m(X) = m_0 + \sum_{v \in \mathcal{P}} m_v(X_v), \quad (2)$$

where m_0 is a constant.

When $|v| = 1$, the function $m_v(X_v)$ corresponds to the main effect of X_v . When $|v| = 2$, i.e. $v = \{a, a'\}$ and $a \neq a'$, the function $m_v(X_v)$ corresponds to the second-order interaction between X_a and $X_{a'}$. And the same holds for $|v| > 2$.

This expansion (2) is unique (Sobol (1993)), all the functions m_v are centered, and they are orthogonal with respect to $L^2(\mathcal{X}, P_X)$.

In the framework of sensitivity analysis, a functional decomposition of the variance could be obtained as follows (Efron and Stein (1981)):

$$\text{Var}(m(X)) = \sum_v \text{Var}(m_v(X_v)).$$

For any group of variables X_v , $v \in \mathcal{P}$, the Sobol indices, introduced by Sobol (1993), are

defined by:

$$S_v = \frac{\text{Var}(m_v(X_v))}{\text{Var}(m(X))}. \quad (3)$$

For each v , S_v expresses the portion of $\text{Var}(m(X))$ explained by X_v .

The classical computation of the Sobol indices is based on the Monte Carlo simulation (see for example: [Sobol \(1993\)](#) for the main effect and interaction indices, and [Saltelli \(2002\)](#) for the main effect and total indices). For models that are expensive to evaluate, the Monte Carlo simulation leads to high computational burden. One solution to this problem is to build a meta model.

A meta model is a function of X that estimates the unknown function m with high precision and presents much lower computational complexity. In the frame work of sensitivity analysis it allows to directly obtain the sensitivity indices.

Several approaches of meta model construction can be found in the literature on the variance-based methods for global sensitivity analysis. The meta model construction based on polynomial chaos expansions ([Wiener \(1938\)](#), [Schoutens \(2000\)](#)) has been presented in [Sudret \(2008\)](#). [Blatman and Sudret \(2011\)](#) build meta models based on sparse polynomial chaos expansion to approximate the Hoeffding decomposition of m and deduce its Sobol indices. They propose a method for truncating the polynomial chaos expansion and an algorithm based on least angle regression for selecting the terms in the expansion.

The principle of the polynomial chaos is to project m onto a basis of orthonormal polynomials. The chaos representation of m , is written as ([Soize and Ghanem \(2004\)](#)):

$$m(X) = \sum_{j=0}^{\infty} h_j \phi_j(X_1, \dots, X_d),$$

where $\{h_j\}_{j=0}^{\infty}$ are the coefficients, and $\{\phi_j(X_1, \dots, X_d)\}_{j=0}^{\infty}$ are multivariate orthonormal polynomials in X that are determined according to the distribution of X . Therefore, for a given distribution of the input variables X , only one family of orthonormal polynomials is considered to construct the functional space. However, this family may not be necessarily the best functional basis to approximate m well. In this approach, the Sobol indices are obtained by summing up the squares of the suitable coefficients.

Another approach to construct meta models is given by Gaussian Process (GP) modelling which has been introduced in the context of sensitivity analysis by [Welch, Buck, Sacks, Wynn, Mitchell, and Morris \(1992\)](#), [Oakley and O'Hagan \(2004\)](#), [Marrel, Iooss, Laurent, and Roustant \(2009\)](#). The principle of GP regression is to consider that the prior knowledge about the function $m(X)$, can be modeled by a GP $\mathcal{Z}(X)$ with a mean $m_{\mathcal{Z}}(X)$ and a covariance kernel $k_{\mathcal{Z}}(X, X')$. To perform the sensitivity analysis from a GP model one may replace the true model $m(X)$ with the mean of the conditional GP, and deduce the sensitivity indices from it. The meta modelling approach based on the polynomial chaos and GP have been reviewed recently by [Le Gratiet, Marelli, and Sudret \(2017\)](#).

The kriging meta models ([Kleijnen \(2007, 2009\)](#)) are similar to the GP meta models, excepting that they do not rely on Bayesian interpretation. The formulation of the kriging meta model provides also analytical formula for the Sobol indices, associated with interval confidence coming from the kriging error ([Le Gratiet, Cannamela, and Iooss \(2014\)](#), [Oakley and O'Hagan \(2004\)](#), [Marrel et al. \(2009\)](#)).

Durrande, Ginsbourger, Roustant, and Carraro (2013) consider a class of functional approximation methods similar to the GP regression and obtain a meta model that satisfies the properties of the Hoeffding decomposition. They propose to approximate m by functions belonging to a RKHS which is constructed as a direct sum of the Hilbert spaces, such that the projection of m onto the RKHS is an approximation of the Hoeffding decomposition of m .

In the regression framework, when the values of $m(X_i)$, $i = 1, \dots, n$ are not observed, one may estimate the function m using non-parametric approaches and deduce the estimators for the Sobol indices from the obtained estimator. In the context of the Gaussian regression model (see Equation (1)), Huet and Taupin (2017) consider the same approximation functional spaces as proposed by Durrande *et al.* (2013), and propose an estimator of a meta model that approximates the Hoeffding decomposition of m . They deduce from this estimated meta model, estimators for the Sobol indices of m .

In this work we consider meta model construction as proposed by Durrande *et al.* (2013). The unknown function m is approximated by its orthogonal projection, denoted by f^* , on a RKHS \mathcal{H} . This space is constructed as a direct sum of Hilbert spaces,

$$\mathcal{H} = 1 + \sum_{v \in \mathcal{P}} \mathcal{H}_v,$$

leading to the Hoeffding decomposition of f^* . The function f^* is defined as the minimizer over the functions $f \in \mathcal{H}$ of the following criteria,

$$E_X(m(X) - f(X))^2. \quad (4)$$

Let $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ be the scalar product in \mathcal{H} . We denote by k and k_v the reproducing kernels associated with the RKHS \mathcal{H} and the RKHS \mathcal{H}_v , respectively. The properties of the RKHS \mathcal{H} insures that any function $f \in \mathcal{H}$, $f : \mathcal{X} \subset \mathbb{R}^d \rightarrow \mathbb{R}$ could be written as the following decomposition:

$$f(X) = \langle f, k(X, \cdot) \rangle_{\mathcal{H}} = f_0 + \sum_{v \in \mathcal{P}} f_v(X_v), \quad (5)$$

where f_0 is a constant, and $f_v : \mathbb{R}^{|v|} \rightarrow \mathbb{R}$ is defined by,

$$f_v(X) = \langle f, k_v(X, \cdot) \rangle_{\mathcal{H}}.$$

For all $v \in \mathcal{P}$, the functions $f_v(X_v)$ are centered and for all $v \neq v'$, the functions $f_v(X_v)$ and $f_{v'}(X_{v'})$ are orthogonal with respect to $L^2(\mathcal{X}, P_X)$. So the decomposition of the function f presented in Equation (5) is its Hoeffding decomposition. As the function f^* belongs to the RKHS \mathcal{H} , it is written as:

$$f^* = f_0^* + \sum_{v \in \mathcal{P}} f_v^*, \quad (6)$$

and each function f_v^* approximates the function m_v in Equation (2). In the decomposition (6) of the function f^* , we have $|\mathcal{P}|$ terms f_v^* that should be estimated. The cardinality of \mathcal{P} is equal to $2^d - 1$ which may be huge since it raises very quickly by increasing d . In order to deal with this problem, one may estimate f^* by a sparse meta model $\hat{f} \in \mathcal{H}$. To this purpose, the estimation of f^* is done on the basis of n observations by minimizing a least square criteria suitably penalized in order to deal both with the non-parametric nature of the problem, and

with the possibly large number of functions that have to be estimated. As we are interested in estimating f^* by a sparse meta model, the penalty function should enforce the sparsity to the obtained solution.

There exists various ways of enforcing sparsity for a minimization (maximization) problem, see for example [Hastie, Tibshirani, and Wainwright \(2015\)](#) for a review. Some methods, such as the sparse additive models (SpAM) procedure ([Ravikumar, Lafferty, Liu, and Wasserman \(2009\)](#), [Liu, Wasserman, and Lafferty \(2009\)](#)), are based on a combination of the l_1 -norm with the empirical L^2 -norm,

$$\|f\|_{n,1} = \sum_{a=1}^d \|f_a\|_n,$$

where

$$\|f_a\|_n^2 = \frac{1}{n} \sum_{i=1}^n f_a^2(X_{ai}),$$

is the squared empirical L^2 -norm for the univariate function f_a . The COSSO method developed by [Lin and Zhang \(2006\)](#), enforces sparsity using a combination of the l_1 -norm with the Hilbert norm,

$$\|f\|_{\mathcal{H},1} = \sum_{a=1}^d \|f_a\|_{\mathcal{H}_a}.$$

Instead of focusing on only one penalty term, one may consider the more general family of estimators, *doubly penalized estimator*, that could be obtained by minimizing a criteria penalized by the following penalty function,

$$\gamma \|f\|_{n,1} + \mu \|f\|_{\mathcal{H},1}, \tag{7}$$

where $\gamma, \mu \in \mathbb{R}$ are the tuning parameters that should be suitably chosen.

[Meier, van de Geer, and Bühlmann \(2009\)](#) proposed a related family of estimators, based on the penalization with the empirical L^2 -norm. Their penalty function is the sum of the sparsity penalty term, $\|f\|_{n,1}$, and a smoothness penalty term. They establish some oracle properties of the empirical risk for estimating the projection of m onto the set of univariate additive functions. [Raskutti, Wainwright, and Yu \(2009, 2012\)](#) derived minimax bounds for sparse additive models. They showed that the *doubly penalized estimator* could reach these bounds for various RKHS families. [Koltchinskii and Yuan \(2008\)](#) analyzed the COSSO estimator and established oracle inequalities on the excess risk assuming that the function m has a sparse representation. They generalized their results to a *doubly penalized estimator* in [Koltchinskii and Yuan \(2010\)](#).

In this paper, we consider a *doubly penalized estimator* of a meta model which approximates the Hoeffding decomposition of m as described in [Huet and Taupin \(2017\)](#). The estimator \hat{f} , called RKHS meta model, is obtained by solving a penalized residual sum of squares minimization. The penalty function (7) is replaced by the sum of the Hilbert norm and the empirical norm of the multivariate functions f_v , $v \in \mathcal{P}$:

$$\gamma \|f\|_n + \mu \|f\|_{\mathcal{H}},$$

with

$$\|f\|_n = \sum_{v \in \mathcal{P}} \|f_v\|_n \quad \text{and} \quad \|f\|_{\mathcal{H}} = \sum_{v \in \mathcal{P}} \|f_v\|_{\mathcal{H}_v}.$$

This procedure, called ridge group sparse, estimates the groups v that are suitable for predicting f^* , and the relationship between f_v^* and X_v for each group. If $\gamma = 0$, then the penalty function contains only the Hilbert norm and the RKHS ridge group sparse procedure reduces to the RKHS group lasso procedure. The estimators for the Sobol indices are deduced from \hat{f} . Our approach makes it possible to estimate the Sobol indices for all groups in the support of the \hat{f} , including the interactions of possibly high order, a point known to be difficult in practice.

The theoretical properties of the estimator based on a ridge group sparse type procedure have been established in the case of the classical non-parametric additive model, i.e. for all v , $|v| = 1$ in decomposition (5), by Raskutti *et al.* (2012). When $v \in \mathcal{P}$ an oracle inequality with respect to the empirical and integrated risks for the RKHS meta model is derived by Huet and Taupin (2017). They obtained an upper bound for the distance between the true function m and its estimation \hat{f} into the RKHS \mathcal{H} .

We propose an R package that implements the approach described in Huet and Taupin (2017), by considering the input variables $X = \{X_1, \dots, X_d\}$ that are mutually independent and uniformly distributed on $\mathcal{X} = [0, 1]^d$, i.e. $X \sim P_X = P_1 \times \dots \times P_d$, with P_a , $a = 1, \dots, d$ representing the uniform law $\mathcal{U}[0, 1]$. This package allows to:

- (1) calculate reproducing kernels and their associated Gram matrices (see section 3.1).
- (2) implement the RKHS ridge group sparse and the RKHS group lasso optimization problems in order to estimate the terms f_v^* in the Hoeffding decomposition of f^* leading to an estimation of the unknown function m (see section 3.2).
- (3) estimate the Sobol indices of the unknown function m (see section 2.4).

To the best of our knowledge there is no other package available to apply our procedure. The **RKHSMetaMod** package is dedicated to the meta model estimation on a RKHS. The convex optimization algorithms used in this package are adapted to take into account the problem of high dimensionality in this context. This package is available from the Comprehensive R Archive Network (CRAN) at <https://cran.r-project.org/web/packages/RKHSMetaMod/>.

In section 2, we present the RKHS ridge group sparse and the RKHS group lasso optimization problems, the approach of constructing RKHS, the choice of the tuning parameters, and the estimation of the Sobol indices. The algorithms used in the **RKHSMetaMod** package to obtain the RKHS meta model are described in section 3. In section 4, we give an overview of the **RKHSMetaMod** functions as well as a brief documentation of them, and in section 5, we illustrate the performances of these functions through four examples.

2. Estimation method

In section 2.1, we describe the RKHS ridge group sparse and the RKHS group lasso optimization problems. In section 2.2, we present the method to construct the RKHS \mathcal{H} . The strategy

of choosing the tuning parameters in the RKHS ridge group sparse algorithm is described in section 2.3, and in section 2.4 we present the calculation of the empirical Sobol indices of RKHS meta model.

2.1. RKHS Ridge group sparse criteria

Let denote by n , the number of observations. The dataset consists of a vector of n observations $Y = (Y_1, \dots, Y_n)$, and a $n \times d$ matrix of features X with components,

$$(X_{ai}, i = 1, \dots, n, a = 1, \dots, d) \in \mathbb{R}^{n \times d}.$$

For some tuning parameters γ and μ , the RKHS ridge group sparse criteria is defined by,

$$\frac{1}{n} \sum_{i=1}^n \left(Y_i - f_0 - \sum_{v \in \mathcal{P}} f_v(X_{vi}) \right)^2 + \gamma \sum_{v \in \mathcal{P}} \|f_v\|_n + \mu \sum_{v \in \mathcal{P}} \|f_v\|_{\mathcal{H}_v}, \quad (8)$$

where X_v represents the matrix of variables corresponding to the v -th group, i.e.

$$X_v = (X_{vi}, i = 1, \dots, n, v \in \mathcal{P}) \in \mathbb{R}^{n \times |\mathcal{P}|},$$

and

$$\|f_v\|_n^2 = \frac{1}{n} \sum_{i=1}^n f_v^2(X_{vi}).$$

The penalty function in the criteria above is the sum of the Hilbert norm and the empirical norm, which allows to select few terms in the additive decomposition of f over sets $v \in \mathcal{P}$. Moreover, the Hilbert norm favours the smoothness of the estimated f_v , $v \in \mathcal{P}$. The minimization of Equation (8) is carried out over a proper subset of the RKHS \mathcal{H} (see [Huet and Taupin \(2017\)](#)).

According to the Representer Theorem ([Kimeldorf and Wahba \(1970\)](#)), for all $v \in \mathcal{P}$, and for some matrix $\theta = (\theta_{vi}, i = 1, \dots, n, v \in \mathcal{P}) \in \mathbb{R}^{n \times |\mathcal{P}|}$ we have,

$$f_v(\cdot) = \sum_{i=1}^n \theta_{vi} k_v(X_{vi}, \cdot).$$

Therefore, the minimization of the functional criteria in Equation (8) over the RKHS \mathcal{H} comes down to the minimization of the parametric criteria in Equation (9) over $f_0 \in \mathbb{R}$, and $\theta_v \in \mathbb{R}^n$ for $v \in \mathcal{P}$:

$$C(f_0, \theta) = \|Y - f_0 I_n - \sum_{v \in \mathcal{P}} K_v \theta_v\|^2 + \sqrt{n} \gamma \sum_{v \in \mathcal{P}} \|K_v \theta_v\| + n \mu \sum_{v \in \mathcal{P}} \|K_v^{1/2} \theta_v\|, \quad (9)$$

where $\|\cdot\|$ is the Euclidean norm in \mathbb{R}^n , and K_v is the $n \times n$ Gram matrix associated with the kernel $k_v(X_v, \cdot)$.

By considering only the second part of the penalty function, $n \mu \sum_{v \in \mathcal{P}} \|K_v^{1/2} \theta_v\|$, in the criteria (9), i.e. set $\gamma = 0$, we obtained the RKHS group lasso criteria:

$$C_g(f_0, \theta) = \|Y - f_0 I_n - \sum_{v \in \mathcal{P}} K_v \theta_v\|^2 + n \mu \sum_{v \in \mathcal{P}} \|K_v^{1/2} \theta_v\|, \quad (10)$$

which is a group lasso criteria (Yuan and Lin (2006a)) up to a scale transformation.

In the **RKHSMetaMod** package, the RKHS ridge group sparse algorithm is initialized using the solutions obtained by solving the RKHS group lasso algorithm. Indeed, the penalty function in the RKHS group lasso criteria (10) insures the sparsity in the solution. Therefore, for a given value of μ , by implementing the RKHS group lasso algorithm (see section 3.2.1), we obtain a RKHS meta model with few terms in its additive decomposition. We denote by $\hat{S}_{\hat{f}_{\text{Group Lasso}}}$ and $\hat{\theta}_{\text{Group Lasso}}$, the support and the coefficients obtained by implementing this algorithm, respectively.

From now on we denote the tuning parameter in the RKHS group lasso algorithm by:

$$\mu_g = \sqrt{n}\mu. \quad (11)$$

2.2. RKHS construction

For all v, v' in \mathcal{P} , the Hoeffding decomposition of m displayed in Equation (2) satisfies,

$$E_X(m_v(X_v)) = E_X(m_v(X_v)m_{v'}(X_{v'})) = 0.$$

The idea is to construct the spaces \mathcal{H} such that any function $f \in \mathcal{H}$ is decomposed as its Hoeffding decomposition (Sobol (2001), Van der Vaart (1998)). So, any function f in the RKHS \mathcal{H} is a candidate to approximate the Hoeffding decomposition of m . The construction of spaces \mathcal{H} , based on ANOVA kernels, was initially given by Durrande *et al.* (2013):

Let $\mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_d$ be a compact subset of \mathbb{R}^d . For each $a \in \{1, \dots, d\}$, we choose a RKHS \mathcal{H}_a and its associated kernel k_a defined on the set $\mathcal{X}_a \subset \mathbb{R}$ such that the two following properties are satisfied:

- (i) $k_a : \mathcal{X}_a \times \mathcal{X}_a \rightarrow \mathbb{R}$ is $P_a \times P_a$ measurable,
- (ii) $E_{P_a} \sqrt{k_a(X_a, X_a)} < \infty$.

The RKHS \mathcal{H}_a may be decomposed as $\mathcal{H}_a = \mathcal{H}_{0a} \oplus \mathcal{H}_{1a}$, where

$$\begin{aligned} \mathcal{H}_{0a} &= \{f_a \in \mathcal{H}_a, E_{P_a}(f_a(X_a)) = 0\}, \\ \mathcal{H}_{1a} &= \{f_a \in \mathcal{H}_a, f_a(X_a) = C\}, \end{aligned}$$

and the kernel k_{0a} associated to the RKHS \mathcal{H}_{0a} is defined as follows (see Berlinet and Thomas-Agnan (2003)):

$$k_{0a}(X_a, X'_a) = k_a(X_a, X'_a) - \frac{E_{U \sim P_a}(k_a(X_a, U))E_{U \sim P_a}(k_a(X'_a, U))}{E_{(U, V) \sim P_a \times P_a} k_a(U, V)}. \quad (12)$$

The ANOVA kernel $k(\cdot, \cdot)$ is defined by:

Let

$$k_v(X_v, X'_v) = \prod_{a \in v} k_{0a}(X_a, X'_a),$$

then

$$k(X, X') = \prod_{a=1}^d (1 + k_{0a}(X_a, X'_a)) = 1 + \sum_{v \in \mathcal{P}} k_v(X_v, X'_v),$$

and its corresponding RKHS,

$$\mathcal{H} = \otimes_{a=1}^d \left(1 \oplus \mathcal{H}_{0a} \right) = 1 + \sum_{v \in \mathcal{P}} \mathcal{H}_v,$$

where \mathcal{H}_v is the RKHS associated with the kernel k_v .

According to this construction, any function $f \in \mathcal{H}$ satisfies Equation (5), which is an approximation of the Hoeffding decomposition of m .

The regularity properties of the RKHS \mathcal{H} constructed as described above, depend on the set of the kernels (k_a , $a = 1, \dots, d$). This method allows to choose different approximation spaces independently of the distribution of the input variables X , by choosing different sets of the kernels. The distribution of X occurs only for the orthogonalization of the spaces \mathcal{H}_v , $v \in \mathcal{P}$. This is one of the main advantages of this method compared to the decomposition based on the truncated polynomial chaos expansion where the smoothness of the approximation is handled only by the choice of the truncation (Blatman and Sudret (2011)).

2.3. Choice of the tuning parameters

In the RKHS ridge group sparse criteria (9), we have two tuning parameters μ and γ to be chosen. To do so, we propose to use a sequence of the tuning parameters, $(\mu, \gamma \geq 0)$, to create a sequence of estimators.

In order to set up the grid of the values of μ , one may set $\gamma = 0$ and find μ_{\max} , the smallest value of μ_g presented in Equation (11), such that the solution to the minimization of the RKHS group lasso problem is $\theta_v = 0$ for all $v \in \mathcal{P}$, by:

$$\mu_{\max} = \max_v \left(\frac{2}{\sqrt{n}} \|K_v^{1/2}(Y - \bar{Y})\| \right). \quad (13)$$

Then

$$\mu_l = \frac{\mu_{\max}}{(\sqrt{n} \times 2^l)}, \quad l \in \{1, \dots, l_{\max}\},$$

could be a grid of values of μ . The grid of values of γ is chosen arbitrary and is done by the user.

For a given grid of values of (μ, γ) a sequence of the RKHS meta models are calculated by solving the RKHS ridge group sparse optimization algorithm (or the RKHS group lasso optimization algorithm if $\gamma = 0$). Then, the obtained estimators are evaluated using a testing dataset $(Y_i^{\text{test}}, X_i^{\text{test}})$, $i = 1, \dots, n^{\text{test}}$. For each value of (μ, γ) in the sequence, let $\hat{f}_{(\mu, \gamma)}$ be the estimation of m , obtained by the learning dataset. Then, the prediction error is calculated by,

$$\text{ErrPred}(\mu, \gamma) = \frac{1}{n^{\text{test}}} \sum_{i=1}^{n^{\text{test}}} (Y_i^{\text{test}} - \hat{f}_{(\mu, \gamma)}(X_i^{\text{test}}))^2,$$

where

$$\hat{f}_{(\mu, \gamma)}(X^{\text{test}}) = \hat{f}_0 + \sum_v \sum_{i=1}^n k_v(X_{vi}, X_v^{\text{test}}) \hat{\theta}_{vi}.$$

We choose the pair $(\hat{\mu}, \hat{\gamma})$ with the smallest value of the prediction error. The model associated with $(\hat{\mu}, \hat{\gamma})$ is the "best" estimator of the unknown function m , and is denoted by $\hat{f} = \hat{f}_{(\hat{\mu}, \hat{\gamma})}$.

In the **RKHSMetaMod** package, the algorithm to calculate a sequence of the RKHS meta models, the value of μ_{\max} , and the prediction error is implemented as `RKHSMetMod()`, `mu_max()`, and `PredErr()` functions, respectively. These functions are described in section 4, and illustrated in Example 5.1, Example 5.3, and Examples 5.1, 5.3, 5.4, respectively.

2.4. Estimation of the Sobol indices

The Sobol indices of the function m are estimated by the Sobol indices of the estimator \hat{f} . According to Equation (3) the Sobol indices of \hat{f} are defined by,

$$S_v = \frac{\text{Var}(\hat{f}_v(X_v))}{\text{Var}(\hat{f}(X))}.$$

The variances of the functions \hat{f}_v , $v \in \mathcal{P}$ are estimated as follows:

Let \hat{f}_v be the empirical mean of $\hat{f}_v(X_{vi})$, $i = 1, \dots, n$, then

$$\widehat{\text{Var}}(\hat{f}_v) = \frac{1}{n-1} \sum_i (\hat{f}_v(X_{vi}) - \hat{f}_v)^2.$$

Besides \hat{f} belongs to the RKHS \mathcal{H} , so we have,

$$\text{Var}(\hat{f}(X)) = \sum_v \text{Var}(\hat{f}_v(X_v)) \quad \text{and} \quad \widehat{\text{Var}}(\hat{f}(X)) = \sum_v \widehat{\text{Var}}(\hat{f}_v(X_v)).$$

For the groups v in the support of \hat{f} , the estimators of the Sobol indices of m are defined by,

$$\hat{S}_v = \frac{\widehat{\text{Var}}(\hat{f}_v(X_v))}{\widehat{\text{Var}}(\hat{f}(X))},$$

and $\hat{S}_v = 0$, for the groups v that do not belong to the support of \hat{f} .

In the **RKHSMetaMod** package, the algorithm to calculate the empirical Sobol indices \hat{S}_v , $v \in \mathcal{P}$ is implemented as a function `SI_emp()`. This function is described in section 4.2 and illustrated in Examples 5.1, 5.3, 5.4.

3. Algorithms

The **RKHSMetaMod** package implements two optimization algorithms: the RKHS ridge group sparse (see Equation (9)) and the RKHS group lasso (see Equation (10)). These algorithms rely on the Gram matrices K_v , $v \in \mathcal{P}$, that have to be positive definite. Therefore, the first and essential step in this package, is to calculate these matrices and insure their positive definiteness. This procedure is detailed in an algorithm that is described in section 3.1.

The second step is to estimate the RKHS meta model. In the **RKHSMetaMod** package we consider two different objectives based on different procedures in order to calculate these estimators:

1. The RKHS meta model with the best prediction quality:

A sequence of values of the tuning parameters (μ, γ) is considered, and the RKHS meta models associated with each pair of values of (μ, γ) is calculated. For $\gamma = 0$, the RKHS meta model is obtained by solving the RKHS group lasso algorithm, while for $\gamma \neq 0$ the RKHS ridge group sparse algorithm is used to calculate the RKHS meta model. The obtained meta models are evaluated by considering a new dataset. The RKHS meta model with minimum value of prediction error is chosen as the "best" estimator.

The algorithms for solving the RKHS ridge group sparse and the RKHS group lasso optimization problems are detailed in sections 3.2.2 and 3.2.1, respectively.

2. The RKHS meta model with at most $qmax$ active groups:

The tuning parameter γ is set as zero. A value of μ for which the number of groups in the solution of the RKHS group lasso problem is equal to $qmax$, is computed. This value will be denoted by μ_{qmax} . Then, the RKHS ridge group sparse algorithm is implemented for a grid of values of $\gamma \neq 0$ and μ_{qmax} . This algorithm is described in section 3.2.3.

3.1. Calculation of the Gram matrices

In the **RKHSMetaMod** package, the algorithm to calculate the Gram matrices K_v , $v \in \mathcal{P}$ is implemented as a function `calc_Kv()`. This algorithm is based on three essential points:

- (1) Set up and modify the chosen kernel:

The available kernels in the **RKHSMetaMod** package are: linear kernel, quadratic kernel, brownian kernel, matern kernel and gaussian kernel. The usual presentation of these kernels is given in Table 1. In order to satisfy the conditions of constructing the RKHS \mathcal{H} (see section 2.2), these kernels should be modified according to Equation (12).

Kernel type	Mathematics formula for $u \in \mathbb{R}^n, v \in \mathbb{R}$	RKHSMetaMod name
Linear	$k_a(u, v) = u^T v + 1$	"linear"
Quadratic	$k_a(u, v) = (u^T v + 1)^2$	"quad"
Brownian	$k_a(u, v) = \min(u, v) + 1$	"brownian"
Matern	$k_a(u, v) = (1 + 2 u - v) \exp(-2 u - v)$	"matern"
Gaussian	$k_a(u, v) = \exp(-2\ u - v\ ^2)$	"gaussian"

Table 1: List of the reproducing kernels used to construct the RKHS \mathcal{H} .

In this package we consider the input variables X that are uniformly distributed on $[0, 1]^d$. If the inputs X are not distributed uniformly, one may modify the calculation of kernels k_{0a} , $a = 1, \dots, d$ (see Equation (12)) with respect to the law of X in the function `calc_Kv()` (see section 4.2) of this package.

- (2) Calculate the Gram matrices K_v for all v :

Firstly, for all $a = 1, \dots, d$ the Gram matrices K_a are calculated using Equation (12), then each K_v is obtained by the Hadamard product of K_a for $a \in v$, i.e.

$$K_v = \bigodot_{a \in v} K_a.$$

(3) Insure the positive definiteness of the matrices K_v :

The output of the function `calc_Kv()` is one of the input arguments of the functions associated with the RKHS group lasso and the RKHS ridge group sparse algorithms. As both of these algorithms rely on the positive definiteness of these matrices, it is mandatory to have $K_v, v \in \mathcal{P}$ that are positive definite. The options, "correction" and "tol", are provided by the function `calc_Kv()` in order to insure the positive definiteness of the matrices $K_v, v \in \mathcal{P}$. Let us briefly explain this part of the algorithm:

For each group $v \in \mathcal{P}$, let $\lambda_{v,i}, i = 1, \dots, n$ be the eigenvalues associated with the matrix K_v . Set $\lambda_{\max} = \max_i \lambda_{v,i}$ and $\lambda_{\min} = \min_i \lambda_{v,i}$. For each matrix K_v

"if $\lambda_{\min} < \lambda_{\max} \times \text{tol}$ ",

then the correction to K_v is done. That is,

"The eigenvalues of K_v are replaced by $\lambda_{v,i} + \text{epsilon}$ ",

where $\text{epsilon} = \lambda_{\max} \times \text{tol}$.

The value of "tol" is set as $1e^{-8}$ by default, but it may be considered smaller (or greater) depending on the chosen kernel.

The function `calc_Kv()` is described in section 4.2 and illustrated in Example 5.3.

3.2. Optimization algorithms

The RKHS meta model is the solution of one of the optimization problems: the minimization of the RKHS group lasso criteria presented in Equation (10) (if $\gamma = 0$), or the minimization of the RKHS ridge group sparse criteria presented in Equation (9) (if $\gamma \neq 0$). The **RKHSMetaMod** package implements RKHS group lasso and RKHS ridge group sparse algorithms via the functions `RKHSgrplasso()` and `pen_MetMod()`, respectively. In the following we present these algorithms in more details.

RKHS group lasso

A popular technique for doing group wise variable selection is group lasso (Yuan and Lin (2006a)). With this procedure, depending on the value of the tuning parameter μ , an entire group of predictors may drop out of the model. An efficient algorithm for solving group lasso problem is block coordinate descent algorithm. Following the idea of Fu (1998), Yuan and Lin (2006b) implemented a block wise descent algorithm for the group lasso penalized least squares, under the condition that the model matrices in each group are orthonormal. A block coordinate (gradient) descent algorithm for solving the group lasso penalized logistic regression is then developed by Meier, van de Geer, and Bühlmann (2008). This algorithm is implemented in the **grplasso** R package available from CRAN at <https://cran.r-project.org/web/packages/grplasso/>. Yang and Zou (2015) proposed an unified algorithm, named groupwise majorization descent, for solving the general group lasso learning problems by assuming that the loss function satisfies a quadratic majorization condition. The implementation of their work is done in the **gglasso** R package available at <https://cran.r-project.org/web/packages/gglasso/> from CRAN.

The **RKHSMetaMod** package applies the block coordinate descent algorithm to the RKHS group lasso problem. In what follows we explain the block coordinate descent algorithm adapted to the RKHS group lasso used in our package.

The minimization of criteria $C_g(f_0, \theta)$ (see Equation (10)) is done along each group v at a time. At each step of the algorithm, the criteria is minimized as a function of the current block's parameters, while the parameters values for the other blocks are fixed to their current values. The procedure is repeated until convergence.

This procedure leads to Algorithm 1. This algorithm is fully described in Appendix A.

Algorithm 1 RKHS group lasso algorithm using block coordinate descent algorithm:

```

1: Set  $\theta_0 = [0]_{|\mathcal{P}| \times n}$ 
2: repeat
3:   Calculate  $f_0 = \operatorname{argmin}_{f_0} C_g(f_0, \theta)$ 
4:   for  $v \in \mathcal{P}$  do
5:     Calculate  $R_v = Y - f_0 - \sum_{v \neq w} K_w \theta_w$ 
6:     if  $\|\frac{2}{\sqrt{n}} K_v^{1/2} R_v\| \leq \mu_g$  then
7:        $\theta_v \leftarrow 0$ 
8:     else
9:        $\theta_v \leftarrow \operatorname{argmin}_{\theta_v} C_g(f_0, \theta)$ 
10:    end if
11:  end for
12: until convergence

```

In the **RKHSMetaMod** package the Algorithm 1 is implemented by the function `RKHSgrplasso()`. This function is described in section 4.2 and illustrated in Example 5.3.

RKHS ridge group sparse

In order to solve the RKHS ridge group sparse optimization problem, we use once again block coordinate descent algorithm. We describe briefly this algorithm in Appendix A, and we refer the reader to the work by Huet and Taupin (2017) for details. The block coordinate descent procedure to solve the RKHS ridge group sparse optimization problem is detailed in Algorithm 2, and is implemented in the **RKHSMetaMod** package, as the function `pen_MetMod()`. This function provides two steps:

Step 1 Initialize the input parameters by the solutions of the RKHS group lasso algorithm for each value of the tuning parameter μ , and run the RKHS ridge group sparse algorithm through active support of the RKHS group lasso solutions until it achieves convergence.

This step is provided in order to decrease the execution time. In fact, instead of implementing the RKHS ridge group sparse algorithm over the set of all groups \mathcal{P} , it is implemented only over the active support obtained by the RKHS group lasso algorithm, $\hat{S}_{\hat{f}_{\text{Group Lasso}}}$.

Step 2 Re-initialize the input parameters with the obtained solutions of Step 1 and implement the RKHS ridge group sparse algorithm through all groups in \mathcal{P} until it achieves convergence.

Algorithm 2 RKHS ridge group sparse algorithm using block coordinate descent algorithm:

- 1: **Step 1:**
 - 2: Set $\theta_0 = \hat{\theta}_{\text{Group Lasso}}$ and $\hat{\mathcal{P}} = \hat{S}_{\hat{f}_{\text{Group Lasso}}}$
 - 3: **repeat**
 - 4: Calculate $f_0 = \operatorname{argmin}_{f_0} C(f_0, \theta)$
 - 5: **for** $v \in \hat{\mathcal{P}}$ **do**
 - 6: Calculate $R_v = Y - f_0 - \sum_{v \neq w} K_w \theta_w$
 - 7: Solve $J^* = \operatorname{argmin}_{\hat{t}_v \in \mathbb{R}^n} \{J(\hat{t}_v), \text{ such that } \|K_v^{-1/2} \hat{t}_v\| \leq 1\}$
 - 8: **if** $J^* \leq \gamma$ **then**
 - 9: $\theta_v \leftarrow 0$
 - 10: **else**
 - 11: $\theta_v \leftarrow \operatorname{argmin}_{\theta_v} C(f_0, \theta)$
 - 12: **end if**
 - 13: **end for**
 - 14: **until** convergence
 - 15: **Step 2:**
 - 16: Implement the same procedure as **Step 1** with $\theta_0 = \hat{\theta}_{\text{old}}$, $\hat{\mathcal{P}} = \mathcal{P} \triangleright \hat{\theta}_{\text{old}}$ is the estimation of θ in **Step 1**.
-

This second step makes it possible to verify that no group is missing in the output of Step 1.

The function `pen_MetMod()` is described in section 4.2 and illustrated in Example 5.3.

RKHS meta model with $qmax$ active groups

By considering some prior information about the data, one may be interested in a meta model with the number of active groups not greater than some " $qmax$ ". To do so,

- Firstly, γ is set to zero in order to find a value μ_{qmax} for which the solution of the RKHS group lasso algorithm, Algorithm 1, contains exactly $qmax$ active groups.
- Then the RKHS ridge group sparse algorithm, Algorithm 2, is implemented by setting the tuning parameter μ equals to μ_{qmax} , and a grid of values of the tuning parameter $\gamma > 0$.

This procedure leads us to Algorithm 3.

As both terms in the penalty function of criteria (9) enforce sparsity to the solution, the estimator obtained by solving the RKHS ridge group sparse associated with the pair of the tuning parameters $(\mu_{qmax}, \gamma > 0)$ may contain a smaller number of groups than the solution of the RKHS group lasso optimization problem (i.e. the RKHS ridge group sparse with $(\mu_{qmax}, \gamma = 0)$). And therefore, the estimated RKHS meta model contains at most " $qmax$ " active groups.

We implement Algorithm 3 in the **RKHSMetaMod** package, as a function `RKHSMetMod_qmax()`. This function is described in section 4.1 and illustrated in Example 5.2.

Algorithm 3 Algorithm to estimate RKHS meta model with at most $qmax$ active groups:

- 1: Calculate $\mu_{\max} = \max_v \frac{2}{\sqrt{n}} \|K_v^{1/2}(Y - \bar{Y})\|$
 - 2: Set $\mu_1 = \mu_{\max}$ and $\mu_2 = \frac{\mu_{\max}}{rat}$ ▷ "rat" is setted by user.
 - 3: **repeat**
 - 4: Implement RKHS group lasso algorithm, Algorithm 1, with $\mu_i = \frac{\mu_1 + \mu_2}{2}$
 - 5: Set $q = |\hat{S}_{\hat{f}_{\text{Group Lasso}}}|$
 - 6: **if** $q > qmax$ **then**
 - 7: Set $\mu_1 = \mu_1$ and $\mu_2 = \mu_i$
 - 8: **else**
 - 9: Set $\mu_1 = \mu_i$ and $\mu_2 = \mu_2$
 - 10: **end if**
 - 11: **until** $q = qmax$ or $i > \text{Num}$ ▷ "Num" is setted by user.
 - 12: Implement RKHS ridge group sparse algorithm, Algorithm 2, with $(\mu = \mu_{qmax}, \gamma > 0)$
-

4. Overview of the RKHSMetaMod functions

In the R environment, one can install and load the **RKHSMetaMod** package by using the following commands:

```
R> install.packages("RKHSMetaMod")
R> library("RKHSMetaMod")
```

The optimization problems in this package are solved using block coordinate descent algorithm which requires various computational algorithms including generalized Newton, Broyden and Hybrid methods. In order to gain the efficiency in terms of the calculation time and be able to deal with high dimensional problems, we use the computationally efficient tools of C++ packages **Eigen** (<http://eigen.tuxfamily.org/>) and **GSL** (<https://www.gnu.org/software/gsl/>) via **RcppEigen** (<https://cran.r-project.org/web/packages/RcppEigen/>) and **RcppGSL** (<https://cran.r-project.org/web/packages/RcppGSL/>) packages. We refer the reader to Eddelbuettel (2013) to have a review of the **RcppEigen** and **RcppGSL** functions.

The complete documentation of **RKHSMetaMod** package is available at <https://cran.r-project.org/web/packages/RKHSMetaMod/RKHSMetaMod.pdf>. Here, we present a brief documentation of some of its main and companion functions in sections 4.1 and 4.2, respectively.

4.1. Main RKHSMetaMod functions

RKHSMetMod() **function:** calculates the Gram matrices K_v , $v \in \mathcal{P}$ associated with a chosen kernel (see Table 1), and fits the solution to the RKHS ridge group sparse (if $\gamma \neq 0$) or the RKHS group lasso problem (if $\gamma = 0$) for each pair of the tuning parameters (μ, γ) . Table 2 gives a summary of all input arguments of the **RKHSMetMod()** function and default values for non mandatory arguments.

The **RKHSMetMod()** function returns a list of l components, with l equals to the number of pairs of the tuning parameters (μ, γ) , i.e. $l = |\text{gamma}| \times |\text{frc}|$. Each component of the list is

Input parameter	Description
Y	Vector of the response observations of size n .
X	Matrix of the input observations with n rows and d columns. Rows correspond to the observations and columns correspond to the variables.
kernel	Character, indicates the type of the kernel (see Table 1) chosen to construct the RKHS \mathcal{H} .
Dmax	Integer, between 1 and d , indicates the maximum order of interactions considered in the RKHS meta model: Dmax= 1 is used to consider only the main effects, Dmax= 2 to include the main effects and the second-order interactions, and so on.
gamma	Vector of non negative scalars, values of the tuning parameter γ in decreasing order. If $\gamma = 0$ the function solves the RKHS group lasso optimization problem and for $\gamma > 0$ it solves the RKHS ridge group sparse optimization problem.
frc	Vector of positive scalars. Each element of the vector sets a value to the tuning parameter μ : $\mu = \mu_{\max}/(\sqrt{n} \times \text{frc})$. The value μ_{\max} (see Equation (13)) is calculated inside the program.
verbose	Logical. Set as TRUE to print: the group v for which the correction of the Gram matrix K_v is done (see section 3.1), and for each pair of the tuning parameters (μ, γ) : the number of current iteration, active groups and convergence criteria. It is set as FALSE by default.

Table 2: List of the input arguments of the `RKHSMetMod()` function.

an instance of the "RKHSMetMod" class. Its three attributes contain all outputs:

- mu: value of the tuning parameter μ (see Equation (9)) if $\gamma > 0$, or $\mu_g = \sqrt{n} \times \mu$ if $\gamma = 0$.
- gamma: value of the tuning parameter γ (see Equation (9)).
- Meta-Model: an RKHS ridge group sparse or RKHS group lasso object associated with the tuning parameters mu and gamma.

RKHSMetMod_qmax() function: calculates the Gram matrices K_v , $v \in \mathcal{P}$ associated with a chosen kernel (see Table 1), determines μ , denoted μ_{qmax} , for which the number of active groups in the RKHS group lasso solution is equal to $qmax$. This function returns an RKHS meta model with at most $qmax$ active groups for each pair of the tuning parameters (μ_{qmax}, γ) (see Algorithm 3). It has the following input arguments:

- Y, X, kernel, Dmax, gamma, verbose (see Table 2).
- qmax: integer, the maximum number of active groups in the obtained solution.
- rat: positive scalar, to restrict the minimum value of μ considered in Algorithm 3,

$$\mu_{\min} = \frac{\mu_{\max}}{(\sqrt{n} \times \text{rat})},$$

where the value of μ_{\max} is given by Equation (13) and is calculated inside the program.

- Num: integer, to restrict the number of different values of the tuning parameter μ to be evaluated in the RKHS group lasso algorithm until it achieves μ_{qmax} . For instance, if Num equals to 1 the program is implemented for three different values of $\mu \in [\mu_{\min}, \mu_{\max}]$:

$$\begin{aligned}\mu_1 &= \frac{(\mu_{\min} + \mu_{\max})}{2} \\ \mu_2 &= \begin{cases} \frac{(\mu_{\min} + \mu_1)}{2} & \text{if } |\hat{S}_{\hat{f}(\mu_1)_{\text{Group Lasso}}}| < qmax \\ \frac{(\mu_1 + \mu_{\max})}{2} & \text{if } |\hat{S}_{\hat{f}(\mu_1)_{\text{Group Lasso}}}| > qmax \end{cases} \\ \mu_3 &= \mu_{\min},\end{aligned}$$

where $|\hat{S}_{\hat{f}(\mu_1)_{\text{Group Lasso}}}|$ is the number of active groups in the solution of the RKHS group lasso algorithm 1 associated with μ_1 .

If Num > 1, the path to cover the interval $[\mu_{\min}, \mu_{\max})$ is detailed in Algorithm 3.

The `RKHSMetMod_qmax()` function returns an instance of the "RKHSMetMod_qmax" class. Its three attributes contain the followings outputs:

- mus: vector of all values of μ_i in Algorithm 3.
- qs: vector with the same length as mus. Each element of the vector shows the number of active groups in the RKHS meta model obtained by solving RKHS group lasso algorithm for an element in mus.
- MetaModel: list of the $l = |\text{gamma}|$ (see input arguments) components. Each component of the list is an instance of the "RKHSMetMod" class for the obtained μ_{qmax} and one value of the tuning parameter γ .

4.2. Companion functions

calc_Kv() function: calculates the Gram matrices K_v , $v \in \mathcal{P}$, for a chosen kernel (see Table 1), and returns their associated eigenvalues and eigenvectors, for $v = 1, \dots, vMax$, with

$$vMax = \sum_{j=1}^{Dmax} \binom{d}{j}.$$

This function has,

- four mandatory input arguments:
 - Y, X, kernel, Dmax (see Table 2).
- three facultative input arguments:
 - correction: logical, set as TRUE to make correction to the matrices K_v (see section 3.1). It is set as TRUE by default.

- verbose: logical, set as TRUE to print: the group for which the correction is done. It is set as TRUE by default.
- tol: scalar to be chosen small, set as $1e^{-8}$ by default.

The `calc_Kv()` function returns a list of two components "kv" and "names.Grp":

- kv: list of vMax components, each component is a list of,
 - Evalues: vector of eigenvalues.
 - Q: matrix of eigenvectors.
- names.Grp: vector of group names of size vMax.

RKHSgrplasso() **function:** fits the solution of the RKHS group lasso problem for a given value of μ_g (see Algorithm 1). It has

- three mandatory input arguments:
 - Y (see Table 2).
 - Kv: list of the eigenvalues and the eigenvectors of the positive definite Gram matrices K_v for $v = 1, \dots, vMax$ and their associated group names (output of the function `calc_Kv()`).
 - mu: positive scalar indicates the value of the tuning parameter μ_g defined in Equation (11).
- two facultative input arguments:
 - maxIter: integer, to set the maximum number of loops through all groups. It is set as 1000 by default.
 - verbose: logical, set as TRUE to print: the number of current iteration, active groups and convergence criteria. It is set as FALSE by default.

This function returns an RKHS group lasso object associated with the tuning parameter μ_g .

mu_max() **function:** calculates the value of the tuning parameter μ_g defined by Equation (11), when the first penalized parameter group enters the model, i.e. the value μ_{max} defined in Equation (13).

It has two mandatory input arguments: the response vector Y , and the list `matZ` of the eigenvalues and eigenvectors of the positive definite Gram matrices K_v for $v = 1, \dots, vMax$. This function returns the μ_{max} value.

pen_MetMod() **function:** fits the solution of the RKHS ridge group sparse optimization problem for each pair of values of the tuning parameters (μ, γ) (see Algorithm 2). This function has

- seven mandatory input arguments:

- Y , γ (see Table 2).
 - Kv : list of the eigenvalues and the eigenvectors of the positive definite Gram matrices K_v for $v = 1, \dots, vMax$ and their associated group names (output of the function `calc_Kv()`).
 - μ : vector of positive scalars. Values of the tuning parameter μ (see Equation (9)) in decreasing order.
 - $resg$: list of the `RKHSgrplasso()` objects associated with each value of the tuning parameter μ , used as initial parameters at Step 1 (see section 3.2.2).
 - γ_v and μ_v : vector of $vMax$ positive scalars. These two inputs are optional, they are provided to associate the weights to the two penalty terms in the RKHS ridge group sparse criteria (9). They set to scalar 0, to consider no weights, i.e. all weights equal to 1.
- three facultative input arguments:
 - $maxIter$: integer, to set the maximum number of loops through initial active groups at Step 1 and maximum number of loops through all groups at Step 2 (see section 3.2.2). It is set as 1000 by default.
 - $verbose$: logical, set as TRUE to print: for each pair of the tuning parameters (μ, γ) : the number of current iteration, active groups and convergence criteria. It is set as FALSE by default.
 - $calcStwo$: logical, set as TRUE to execute Step 2 (see section 3.2.2). It is set as FALSE by default.

The function `pen_MetMod()` returns an RKHS ridge group sparse object associated with each pair of the tuning parameters (μ, γ) .

PredErr() function: calculates the prediction errors for the obtained RKHS meta models by considering a testing dataset. It has eight mandatory input arguments:

- X , γ , $kernel$, $Dmax$ (see Table 2).
- XT : matrix of observations of the testing dataset with n^{test} rows and d columns.
- YT : vector of response observations of the testing dataset of size n^{test} .
- μ : vector of positive scalars. Values of the tuning parameter μ (see Equation (9)) in decreasing order.
- res : list of the estimated RKHS meta models for the learning dataset associated with the tuning parameters (μ, γ) (it could be the output of one of the functions `RKHSMetMod()`, `RKHSMetMod_qmax()` or `pen_MetMod()`).

Note that, the same kernel and $Dmax$ should be chosen as the ones used for the learning dataset.

The function `PredErr()` returns a matrix of the prediction errors. Each element of the matrix corresponds to the prediction error of one RKHS meta model in "res".

SI_emp() **function:** calculates the empirical Sobol indices for an input or a group of inputs. It has two input arguments:

- res: list of the estimated meta models using RKHS ridge group sparse or RKHS group lasso algorithms (it could be the output of one of the functions `RKHSMetMod()`, `RKHSMetMod_qmax()` or `pen_MetMod()`).
- ErrPred: matrix or NULL. If matrix, each element of the matrix corresponds to the prediction error of an RKHS meta model in "res" (output of the function `PredErr()`). Set as NULL by default.

The empirical Sobol indices are then calculated for each RKHS meta model in "res", and a list of vectors of the Sobol indices is returned.

If the argument "ErrPred" is the matrix of the prediction errors, the vector of empirical Sobol indices is returned for the "best" RKHS meta model in the "res".

5. RKHSMetaMod through examples

Recall our model, $Y = m(X) + \sigma\varepsilon$, with errors ε that are distributed identically and independently with centered gaussian law, $\varepsilon_i \sim \mathcal{N}(0, 1)$, and $\sigma > 0$. We consider the g-function of Sobol (Saltelli, Chan, and Scott (2009)) for which the Sobol indices could be expressed analytically. The g-function is defined over $[0, 1]^d$ by,

$$m(X) = \prod_{a=1}^d \frac{|4x_a - 2| + c_a}{1 + c_a}, c_a > 0. \quad (14)$$

Set $c_1 = 0.2$, $c_2 = 0.6$, $c_3 = 0.8$ and $(c_a)_{a>3} = 100$. With these values of coefficients c_a , the variables X_1, X_2 and X_3 explain 99.99% of the variance of the function $m(X)$ (Durrande *et al.* (2013)).

In this section, we present four examples. In all examples the value of Dmax is set as three. Example 5.1 illustrates the use of the `RKHSMetMod()` function by considering three different kernels, "matern", "brownian", and "gaussian" (see Table 1), and three datasets of $n \in \{50, 100, 200\}$ observations and $d = 5$ input variables. In Example 5.2, the function `RKHSMetMod_qmax()` is illustrated for dataset of $n = 500$ observations and $d = 10$ input variables. The larger datasets with $n \in \{1000, 2000, 5000\}$ observations and $d = 10$ input variables are studied in Examples 5.3 and 5.4.

In each example, two independent datasets: (X, Y) to estimate the meta models, and (XT, YT) to estimate the prediction error, are generated. The design matrices X and XT are the Latin Hypercube Samples of the inputs that are generated using `maximinLHS()` function of the package `lhs` available at <https://CRAN.R-project.org/package=lhs>. The response variables Y and YT are calculated as $Y = m(X) + \sigma\varepsilon$ and $YT = m(XT) + \sigma\varepsilon_T$, where ε and ε_T are distributed independently according to the centered Gaussian distribution with variance equals to one and $\sigma = 0.2$.

Example 5.1 *RKHS meta model estimation using `RKHSMetMod()` function:*

We set $n \in \{50, 100, 200\}$, $d = 5$, and we generate a n point `maximinLHS()` over $[0, 1]^5$. In this example, we consider a grid of five values for each of the tuning parameters μ and γ as:

$$\mu_{(1:5)} = \frac{\mu_{max}}{(\sqrt{n} \times 2^{(2:6)})}, \quad \gamma_{(1:5)} = (0.2, 0.1, 0.01, 0.005, 0).$$

The experiment is repeated $N_r = 50$ times. At each repetition, the RKHS meta models associated with the pair of the tuning parameters (μ, γ) are estimated using the `RKHSMetMod()` function:

```
R> Dmax <- 3
R> gamma <- c(0.2, 0.1, 0.01, 0.005, 0)
R> frc <- 1/(0.5^(2:6))
R> res <- RKHSMetMod(Y, X, kernel, Dmax, gamma, frc, FALSE)
```

These meta models are evaluated using a testing dataset. The prediction errors are computed for them using the `PredErr()` function. The RKHS meta model with minimum prediction error is chosen to be the "best" estimator for the model. Finally, the Sobol indices are computed for the "best" RKHS meta model using the function `SI_emp()`:

```
R> l <- length(gamma)
R> mu <- vector(); for(i in 1:length(frc)){mu[i] <- res[[i-1]*l+1]}$mu}
R> Err <- PredErr(X, XT, YT, mu, gamma, res, kernel, Dmax)
R> SI_emp(res, Err)
```

The performances of this method for estimating a meta model are evaluated by a third dataset $(m(X_i^{third}), X_i^{third})$, $i = 1, \dots, N$, with $N = 1000$. The global prediction error is calculated as follows:

Let $\hat{f}_r(\cdot)$ be the "best" RKHS meta model obtained in the repetition r , $r = 1, \dots, N_r$, then

$$GPE = \frac{1}{N_r} \sum_{r=1}^{N_r} \frac{1}{N} \sum_{i=1}^N (\hat{f}_r(X_i^{third}) - m(X_i^{third}))^2.$$

The values of GPE obtained for different kernels and values of n are given in Table 3.

n	50	100	200
GPE_m	0.13	0.07	0.03
GPE_b	0.14	0.10	0.05
GPE_g	0.15	0.11	0.07

Table 3: Example 5.1: The columns of the table correspond to the different datasets with $n \in \{50, 100, 200\}$ and $d = 5$. Each line of the table, from up to down, gives the value of GPE obtained for each dataset associated with the "matern", "brownian" and "gaussian" kernels, respectively.

As expected the value of GPE decreases as n increases. The lowest values of GPE are obtained when using the "matern" kernel.

In order to sum up the behaviour of our procedure for estimating the Sobol indices, we estimate the mean square error (MSE) as follows:

Let

$$b_v^2 = (\hat{S}_{v,\cdot} - S_v)^2 \quad \text{and} \quad w_v^2 = \frac{1}{N_r} \sum_{r=1}^{N_r} (\hat{S}_{v,r} - \hat{S}_{v,\cdot})^2,$$

where for each group v , S_v denotes the true value of the Sobol indices of group v , $\hat{S}_{v,r}$ is the empirical Sobol indices in repetition r , and

$$\hat{S}_{v,\cdot} = \frac{1}{N_r} \sum_{r=1}^{N_r} \hat{S}_{v,r}.$$

Then,

$$MSE = \sum_v (b_v^2 + w_v^2).$$

The obtained values of MSE for different kernels and values of n , are given in Table 4.

n	50	100	200
MSE_m	75.1	46.7	28.2
MSE_b	110.7	85.0	41.1
MSE_g	78.2	94.7	67.0

Table 4: Example 5.1: The columns of the table correspond to the different datasets with $n \in \{50, 100, 200\}$ and $d = 5$. Each line of the table, from up to down, gives the value of MSE obtained for each dataset associated with the "matern", "brownian" and "gaussian" kernels, respectively.

As expected, the values of MSE are smaller for larger values of n . The smallest values are obtained when using "matern" kernel.

The means of the empirical Sobol indices of the "best" RKHS meta models through all repetitions for $n = 200$ and "matern" kernel are displayed in Table 5.

v	{1}	{2}	{3}	{1, 2}	{1, 3}	{2, 3}	{1, 2, 3}	sum
S_v	43.3	24.3	19.2	5.63	4.45	2.50	0.57	99.98
$\hat{S}_{v,\cdot}$	46.1	26.3	20.6	2.9	2.2	1.1	0.0	99.2

Table 5: Example 5.1: The first line of the table gives the true values of the Sobol indices $\times 100$ greater than 10^{-2} . The second line gives the mean of the estimated empirical Sobol indices $\times 100$ greater than 10^{-2} calculated over fifty simulations for $n = 200$ and "matern" kernel. The sum of the Sobol indices is displayed in the last column.

It appears that the estimated Sobol indices are close to the true ones, nevertheless they are over estimated for the main effects, i.e. groups $v \in \{\{1\}, \{2\}, \{3\}\}$, and under estimated for the interactions of order two and three, i.e. groups $v \in \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\}\}$.

Note that, the strategy of choosing the tuning parameters is based on the minimization of the prediction error of the estimated meta model, which may not minimize the error of estimating the Sobol indices.

Taking into account the results obtained for this Example 5.1, we continue the calculations in the rest of the examples using only the "matern" kernel.

Example 5.2 Estimate the meta models with at most "qmax" active groups:

We generate a n point `maximinLHS()` over $[0, 1]^d$ with $n = 500$ and $d = 10$. According to the true values of the Sobol indices presented in Table 5, we notice that the main factors X_1, X_2 , and X_3 explain almost all of the variability in the model. So, one may be interested in estimating the function $m(X)$ (see Equation (14)) by a meta model that includes at most three active groups (the main effects only). We consider five values of the tuning parameter $\gamma_{(1:5)} = (0.2, 0.1, 0.01, 0.005, 0)$. We aim to find a $\mu_{qmax=3}$, such that the RKHS meta model associated with $(\mu_{qmax=3}, \gamma_i = 0)$ contains three active groups. Then, we estimate the RKHS meta models for $(\mu_{qmax=3}, \gamma_i)$, $i = 1, \dots, 5$ that contain at most three active groups. To this purpose, we use the `RKHSMetMod_qmax()` function with

- "rat"= 100: the minimum value of μ considered in the algorithm is then

$$\mu_{min} = \frac{\mu_{max}}{(\sqrt{n} \times 100)},$$

- "Num"= 10: the maximum number of values of $\mu \in [\mu_{min}, \mu_{max})$ to be evaluated is equal to twelve (see Algorithm 3).

```
R> Dmax <- 3
R> res <- RKHSMetMod_qmax(Y, X, kernel, Dmax, gamma, qmax, Num, rat, FALSE)
```

The RKHS meta models are estimated for the obtained value of μ_{qmax} and different values of the tuning parameter γ :

```
R> for(i in 1:length(gamma)){
+ print(paste("In meta model ", i))
+ print(paste("the value of mu is: ", res$MetaModel[[i]]$mu,
+ "and the value of gamma is: ", res$MetaModel[[i]]$gamma))
+ print("the active groups are: ")
+ print(res$MetaModel[[i]]$`Meta-Model`$Nsupp)
+ }
[1] "In meta model 1"
[1] "the value of mu is: 0.093 and the value of gamma is: 0.2"
[1] "the active groups are: "
[1] "v1." "v2." "v3."
[1] "In meta model 2"
[1] "the value of mu is: 0.093 and the value of gamma is: 0.1"
[1] "the active groups are: "
[1] "v1." "v2." "v3."
[1] "In meta model 3"
[1] "the value of mu is: 0.093 and the value of gamma is: 0.01"
[1] "the active groups are: "
[1] "v1." "v2." "v3."
[1] "In meta model 4"
[1] "the value of mu is: 0.093 and the value of gamma is: 0.005"
```



```
[1] "the active groups are: "
[1] "v1." "v2." "v3."
[1] "In meta model 5"
[1] "the value of mu is: 2.083 and the value of gamma is: 0"
[1] "the active groups are: "
[1] "v1." "v2." "v3."
```

The value of the tuning parameter $\mu_{q_{max}=3}$ is equal to 0.093.

Let us comment the outputs of the function `RKHSMetMod_qmax()`: for $\gamma = 0$ the value "mu" corresponds to the value of μ_g defined in Equation (11), i.e.

$$\mu_g = \sqrt{n} \times 0.093 = 2.083,$$

while for $\gamma \neq 0$ it corresponds to the value of μ in the RKHS ridge group sparse criteria (9).

For each pair of the tuning parameters $(\mu_{q_{max}}, \gamma_i)$, $i = 1, \dots, 5$, the estimated RKHS meta model contains three groups. As expected, the groups associated with X_1, X_2, X_3 are "v1.", "v2.", and "v3.", that are active in the estimators obtained.

Example 5.3 *A time saving trick to obtain the "optimal" tuning parameters when dealing with larger datasets:*

We take $n = 1000$, $d = 10$, and we generate a 1000 point `maximinLHS()` over $[0, 1]^{10}$. Firstly, the eigenvalues and eigenvectors of the positive definite matrices K_v , and the value of μ_{max} is computed using functions `calc_Kv()` and `mu_max()`, respectively:

```
R> Dmax <- 3
R> Kv <- calc_Kv(X, kernel, Dmax, TRUE, TRUE)
R> mumax <- mu_max(Y, Kv$kv)
```

Then we consider the two following steps:

1. Set $\gamma = 0$ and,

$$\mu^{(1:9)} = \frac{\mu_{max}}{(\sqrt{n} \times 2^{(2:10)})}.$$

Calculate an RKHS meta model for each value of $\mu_g = \mu \times \sqrt{n}$ using the function `RKHSgrplasso()`. Gather all the RKHS meta models obtained by solving RKHS group lasso algorithm in a list, `res_g` (while this job could be done with the function `RKHSMetMod()` by setting $\gamma = 0$, in this example we use the function `RKHSgrplasso()` in order to avoid the re-calculation of K_v 's at the next step). Thereafter, the prediction error for each estimator in the `res_g` is calculated using the function `PredErr()`. We denote by μ_i the value of μ with the smallest error of prediction in this step.

Let us implement this step:

For a grid of values of μ_g , a sequence of the RKHS meta models are calculated, and gathered in a list:

```
R> mu_g <- c(mumax*0.5^(2:10))
R> resg <- list() ; res_g <- list()
R> for(i in 1:length(mu_g)){
  resg[[i]] <- RKHSgrplasso(Y,Kv, mu_g[i] , 1000, FALSE)
  res_g[[i]] <- list("mu_g"=mu_g,"gamma"=0,"MetaModel"=resg[[i]])
}
```

Output `res_g` contains nine RKHS meta models and they are evaluated using a testing dataset:

```
R> gamma <- c(0)
R> Err_g <- PredErr(X,XT,YT,mu_g,gamma,res_g,kernel,Dmax)
```

The prediction errors of the RKHS meta models obtained in this step are displayed in Table 6.

μ_g	1.304	0.652	0.326	0.163	0.081	0.040	0.020	0.010	0.005
$\gamma = 0$	0.196	0.156	0.144	0.097	0.063	0.055	0.056	0.063	0.073

Table 6: Example 5.3: Obtained prediction errors in step 1.

It appears that the minimum prediction error corresponds to the solution of the RKHS group lasso algorithm with $\mu_g = 0.040$, so $\mu_i = 0.040/\sqrt{n}$.

- Choose a smaller grid of values of μ , $(\mu_{(i-1)}, \mu_i, \mu_{(i+1)})$, and set a grid of values of $\gamma > 0$. Estimate the RKHS meta models associated with each pair of the tuning parameters (μ, γ) by the function `pen_MetMod()`. Calculate the prediction error for the new sequence of the RKHS meta models using the function `PredErr()`. Compute the empirical Sobol indices for the "best" estimator.

Let us go back to the implementation of the example and apply this step 2:

The grid of values of μ in this step is,

$$\left(\frac{0.081}{\sqrt{n}}, \frac{0.040}{\sqrt{n}}, \frac{0.020}{\sqrt{n}}\right).$$

We set $\gamma_{(1:4)} = (0.2, 0.1, 0.01, 0.005)$, and we estimate the RKHS meta models for this new grid of values of (μ, γ) using `pen_MetMod()` function:

```
R> mu <- c(mu_g[5], mu_g[6], mu_g[7])/sqrt(n)
R> gamma <- c(0.2, 0.1, 0.01, 0.005)
R> res <- pen_MetMod(Y,Kv,gamma,mu,resg,0,0)
```

The output "res" is a list of twelve RKHS meta models. These meta models are evaluated using a new dataset, and their prediction errors are displayed in Table 7.

The minimum prediction error is associated with the pair $(0.020/\sqrt{n}, 0.01)$, and the "best" RKHS meta model is then $\hat{f}_{(0.020/\sqrt{n}, 0.01)}$.

The performances of this procedure for estimating the Sobol indices is evaluated using the relative error (RE) defined as follows:

μ	$0.081/\sqrt{n}$	$0.040/\sqrt{n}$	$0.020/\sqrt{n}$
$\gamma = 0.2$	0.152	0.130	0.119
$\gamma = 0.1$	0.097	0.079	0.071
$\gamma = 0.01$	0.065	0.054	0.052
$\gamma = 0.005$	0.064	0.054	0.053

Table 7: Example 5.3: Obtained prediction errors in step 2.

For each v , let S_v be the true value of the Sobol indices displayed in Table 5 and \hat{S}_v be the estimated empirical Sobol indices. Then

$$RE = \sum_v \frac{|\hat{S}_v - S_v|}{S_v}. \quad (15)$$

In Table 8 the estimated empirical Sobol indices, their sum, and the value of RE are displayed.

v	{1}	{2}	{3}	{1, 2}	{1, 3}	{2, 3}	{1, 2, 3}	sum	RE
\hat{S}_v	42.9	25.5	20.8	4.4	3.8	2.1	0.0	99.5	1.68

Table 8: Example 5.3: The estimated empirical Sobol indices $\times 100$ greater than 10^{-2} . The last two columns show $\sum_v \hat{S}_v$ and RE, respectively.

The RE for each group v is smaller than 1.68%, so the estimated Sobol indices in this example are very close to the true values of the Sobol indices displayed in the first row of Table 5. We also obtained the significant values of the Sobol indices for interactions of order two.

Example 5.4 Dealing with larger datasets:

We consider $n \in \{2000, 5000\}$, $d = 10$, and we generate a n point `maximinLHS()` over $[0, 1]^{10}$. In order to obtain one RKHS meta model associated with one pair of the tuning parameters (μ, γ) , the number of coefficients to be estimated is equal to:

$$n \times \sum_{i=1}^{Dmax} \binom{d}{i} = n \times 175.$$

Table 9 gives the execution time for different functions used throughout the Examples 5.1-5.4.

As we can see, the execution time increases fastly as n increases.

In Figure 1 the plot of the logarithm of the time versus the logarithm of n is displayed for the functions `calc_Kv()`, `mu_max()`, `RKHSgrplasso()` and `pen_MetMod()`. It appears that, the algorithms of these functions are of polynomial time $O(n^\alpha)$ with $\alpha \simeq 3$ for the functions `calc_Kv()` and `mu_max()`, and $\alpha \simeq 2$ for the functions `RKHSgrplasso()` and `pen_MetMod()`.

Taking into account the results obtained for the prediction error and the values of $(\hat{\mu}, \hat{\gamma})$ in Example 5.3, in this example we consider two values of the tuning parameter

$$\mu = \left(\frac{\mu_{max}}{(\sqrt{n} \times 2^7)}, \frac{\mu_{max}}{(\sqrt{n} \times 2^8)} \right),$$

(n, d)	calc_Kv()	mu_max()	RKHSgrplasso()	pen_MetMod()	$ S_{\hat{f}} $	sum
(100,5)	0.09s	0.01s	1s	2s	18	$\sim 3s$
			2s	3s	19	$\sim 5s$
(500,10)	33s	9s	247s	333s	39	$\sim 10min$
			599s	816s	64	$\sim 24min$
(1000,10)	197s	53s	959s	1336s	24	$\sim 42min$
			2757s	4345s	69	$\sim 2h$
(2000,10)	1498s	420s	3984s	4664s	12	$\sim 2h:56min$
			12951s	22385s	30	$\sim 10h:20min$
(5000,10)	34282s	6684s	38957s	49987s	11	$\sim 36h:05min$
			99221s	111376s	15	$\sim 69h:52min$

Table 9: Example 5.4: The kernel used is "matern". The execution time for the functions `RKHSgrplasso()` and `pen_MetMod()` is displayed in each row for two pair of values of tuning parameters ($\mu_1 = \mu_{max}/(\sqrt{n} \times 2^7)$, $\gamma = 0.01$) on up, and ($\mu_2 = \mu_{max}/(\sqrt{n} \times 2^8)$, $\gamma = 0.01$) on below. In the column $|S_{\hat{f}}|$, the number of the active groups associated with each estimated RKHS meta model is displayed.

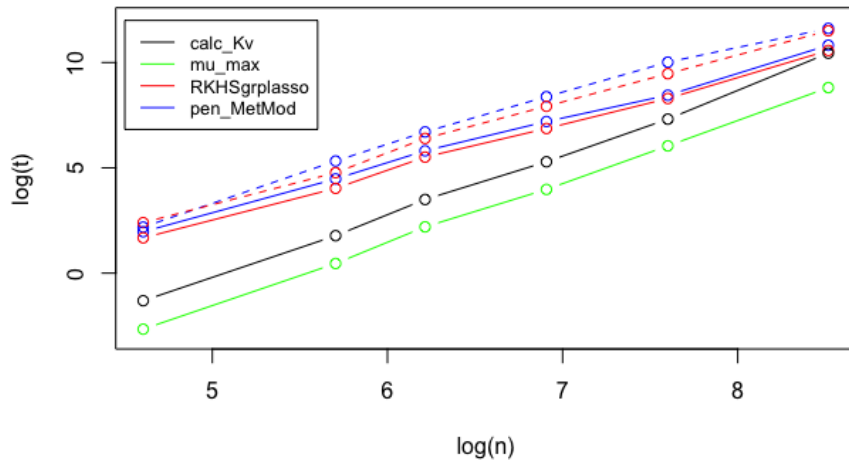


Figure 1: Example 5.4: Timing plot for $d = 10$, $n \in \{100, 300, 500, 1000, 2000, 5000\}$, and different functions of the **RKHSMetaMod** package. The execution time for the functions `RKHSgrplasso()` and `pen_MetMod()` is displayed for two pair of values of tuning parameters ($\mu_1 = \mu_{max}/(\sqrt{n} \times 2^7)$, $\gamma = 0.01$) in solid lines, and ($\mu_2 = \mu_{max}/(\sqrt{n} \times 2^8)$, $\gamma = 0.01$) in dashed lines.

and one value of the tuning parameter $\gamma = 0.01$. The RKHS meta models associated with the pair of values (μ_i, γ) , $i = 1, 2$ are estimated using the `RKHSMetaMod()` function:

```
R> Dmax <- 3
R> frc <- 1/(0.5^(7:8))
```

```
R> gamma <- c(0.01)
R> res <- RKHSMetaMod(Y,X, kernel, Dmax, gamma, frc, FALSE)
```

The prediction error and the empirical Sobol indices are then calculated for the obtained meta models using the functions `PredErr()` and `SI_emp()`:

```
R> mu <- vector(); for(i in 1:length(frc)){mu[i] <- res[[i-1]*1+1]}$mu}
R> Err <- PredErr(X,XT, YT,mu,gamma, res, kernel,Dmax)
R> SI <- SI_emp(res, NULL)
```

The result of the prediction errors associated with the obtained estimators for two different values of n are displayed in Table 10.

n	$(\mu_{max}/(\sqrt{n} \times 2^7), \gamma)$	$(\mu_{max}/(\sqrt{n} \times 2^8), \gamma)$
2000	0.052	0.049
5000	0.048	0.046

Table 10: Example 5.4: Obtained prediction errors.

For n equals to 5000 we get smaller values of the prediction error, so as expected, the prediction quality improves by increasing the number of the observations n . Table 11 gives the estimated empirical Sobol indices as well as their sum and the values of RE (see Equation (15)).

n	v	{1}	{2}	{3}	{1, 2}	{1, 3}	{2, 3}	{1, 2, 3}	sum	RE
2000	$\hat{S}_{v;(\mu_1, \gamma)}$	45.5	24.7	21.0	3.9	3.0	1.6	0.0	99.7	2.1
	$\hat{S}_{v;(\mu_2, \gamma)}$	45.3	25.0	19.6	4.3	3.6	1.8	0.0	99.6	1.8
5000	$\hat{S}_{v;(\mu_1, \gamma)}$	44.7	25.3	20.0	4.5	3.4	1.9	0.0	99.8	1.7
	$\hat{S}_{v;(\mu_2, \gamma)}$	43.7	24.9	19.5	5.4	3.9	2.3	0.0	99.7	1.2

Table 11: Example 5.4: The estimated empirical Sobol indices $\times 100$ greater than 10^{-2} associated with each estimated RKHS meta model is printed. The last two columns show $\sum_v \hat{S}_v$ and RE, respectively. We have $\mu_1 = \mu_{max}/(\sqrt{n} \times 2^7)$, $\mu_2 = \mu_{max}/(\sqrt{n} \times 2^8)$ and $\gamma = 0.01$.

Comparing the values of RE, we can see that the empirical Sobol indices are better estimated for n equals to 5000, so as expected, the estimation of the Sobol indices is better for larger values of n .

In Figure 2 the result of the prediction quality and the Sobol indices for dataset with n equals to 5000, d equals to 10, and (μ_2, γ) are displayed.

The line $y = x$ in red crosses the cloud of points as long as the values of the g-function are smaller than three. When the values of the g-function are greater than three, the estimator \hat{f} tends to under estimate the g-function.

6. Summary and discussion

This paper proposed an R package, called **RKHSMetaMod**, that allows to estimate a meta model and the Sobol indices of a complex model m in the Gaussian regression framework. This meta model belongs to a reproducing kernel Hilbert space constructed as a direct sum of the

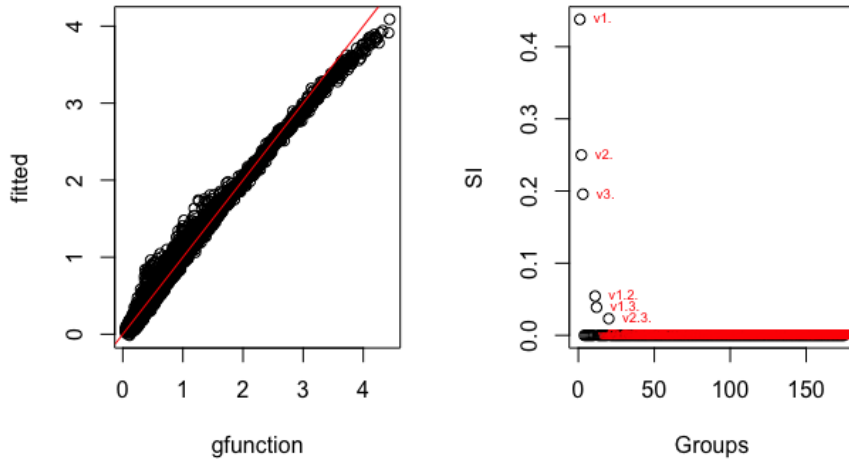


Figure 2: On the left, the RKHS meta model versus the g-function is plotted. On the right, the empirical Sobol indices in the y axis and $v\text{Max}=175$ groups in the x axis are displayed.

Hilbert spaces. The estimation of the meta model is carried out via a penalized least squares minimization allowing both to select and estimate the terms in the Hoeffding decomposition, and therefore, to select the Sobol indices that are non-zero and estimate them. It makes possible to estimate Sobol indices of high order, a point known to be difficult in practice.

Using the convex optimization tools, **RKHSMetaMod** package implements two optimization algorithms: the minimization of the RKHS ridge group sparse criteria (9) and the RKHS group lasso criteria (10). Both of these algorithms rely on the Gram matrices K_v , $v \in \mathcal{P}$ and their positive definiteness.

Currently, the package considers only uniformly distributed variables X . If one is interested by another distribution of the input variables X , it suffices to modify the calculation of the kernels k_{0a} , $a = 1, \dots, d$ (see Equation (12)) in the function `calc_Kv()` of this package.

The available kernels in the **RKHSMetaMod** package are: linear kernel, quadratic kernel, brownian kernel, matern kernel and gaussian kernel (see Table 1). Regarding to the problem under study, one may consider another kernel and add it easily to the list of the kernels in the `calc_Kv()` function. Indeed, the choice of different kernels allows to consider different spaces of approximations and choose the one that gives the best result.

For the large values of n and d the calculation and storage of the eigenvalues and the eigenvectors of all Gram matrices K_v , $v \in \mathcal{P}$ requires a lot of time and a very large amount of memory. In order to optimize the execution time and also the storage memory, almost all of the functions in this package are written using C++ libraries **GSL** and **Eigen**. They are then interfaced with the R environment in order to propose an user friendly package.

This package deals with small and large datasets and allows to obtain an estimator with high prediction quality for the model under study as well as good estimation of its Sobol indices (see Examples 5.1-5.4).

The strategy of choosing the tuning parameters in this package is based on the minimization of the prediction error of the estimated meta model, the prediction error being estimated using a testing dataset. The "best" estimator is selected in terms of the prediction quality, and the Sobol indices are deduced from it. Another procedure of choosing the tuning parameters in order to insure the good prediction quality is described in [Huet and Taupin \(2017\)](#).

If one is specially interested in the estimation of the Sobol indices, an alternative to our approach could be to calculate the tuning parameters which minimize the prediction error of the Sobol indices.

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A. More technical details

Preliminary A.1 For $F(x) = \|Ax\|$, where A is a symmetric matrix that not depends on x , we have,

$$\begin{aligned} \partial F(x) &= \left\{ \frac{A^2 x}{\|Ax\|} \right\} && \text{if } x \neq 0, \\ \partial F(x) &= \{w \in \mathbb{R}^n, \|A^{-1}w\| \leq 1\} && \text{if } x = 0. \end{aligned}$$

Preliminary A.2 Let $F : \mathbb{R}^n \rightarrow \mathbb{R}$ be a convex function. we have the following first order optimality condition:

$$\hat{x} \in \operatorname{argmin}_{x \in \mathbb{R}^n} F(x) \Leftrightarrow 0 \in \partial F(\hat{x}).$$

This follows from the fact that $F(y) \geq F(\hat{x}) + \langle 0, y - \hat{x} \rangle$ for all $y \in \mathbb{R}^n$ in both cases (Giraud (2014)).

RKHS group lasso algorithm

We consider the minimization of the RKHS group lasso criteria given by,

$$C_g(f_0, \theta) = \|Y - f_0 I_n - \sum_{v \in \mathcal{P}} K_v \theta_v\|^2 + \sqrt{n} \mu_g \sum_{v \in \mathcal{P}} \|K_v^{1/2} \theta_v\|.$$

We begin with the constant term f_0 . The ordinary first derivative of the function $C_g(f_0, \theta)$ at f_0 is equal to:

$$\frac{\partial C_g}{\partial f_0} = -2 \sum_{i=1}^n (Y_i - f_0 I_n - \sum_{v \in \mathcal{P}} K_v \theta_v)_i,$$

and therefore,

$$\hat{f}_0 = \frac{1}{n} \sum_{i=1}^n Y_i - \frac{1}{n} \sum_i \sum_v (K_v \theta_v)_i,$$

where $(K_v \theta_v)_i$ denotes the i -th component of $K_v \theta_v$.

Next step is to calculate,

$$\hat{\theta} = \operatorname{argmin}_{\theta \in \mathbb{R}^n \times |\mathcal{P}|} C_g(f_0, \theta).$$

Since $C_g(f_0, \theta)$ is convex and separable, we use a block coordinate descent algorithm, group v by group v . In the following, we fix a group v , and we find the minimizer of $C_g(f_0, \theta)$ with respect to θ_v for given values of f_0 and θ_w , $w \neq v$. Set

$$C_{g,v}(f_0, \theta_v) = \|R_v - K_v \theta_v\|^2 + \sqrt{n} \mu_g \|K_v^{1/2} \theta_v\|,$$

where

$$R_v = Y - f_0 - \sum_{w \neq v} K_w \theta_w. \tag{16}$$

We aim to minimize $C_{g,v}(f_0, \theta_v)$ with respect to θ_v . Let $\partial C_{g,v}$ be the sub-differential of $C_{g,v}(f_0, \theta_v)$ with respect to θ_v :

$$\partial C_{g,v}(f_0, \theta) = \{-2K_v(R_v - K_v \theta_v) + \sqrt{n} \mu_g t_v \quad : \quad t_v \in \partial \|K_v^{1/2} \theta_v\|\}.$$

The first order optimality condition (see Preliminary (A.2)) ensures the existence of $\hat{t}_v \in \partial\|K_v^{1/2}\theta_v\|$ fulfilling,

$$-2K_v(R_v - K_v\theta_v) + \sqrt{n}\mu_g\hat{t}_v = 0. \quad (17)$$

Using the sub-differential definition (see Preliminary A.1) we obtain,

$$\partial\|K_v^{1/2}\theta_v\| = \left\{ \frac{K_v\theta_v}{\|K_v^{1/2}\theta_v\|} \right\} \quad \text{if } \theta_v \neq 0,$$

and,

$$\partial\|K_v^{1/2}\theta_v\| = \{\hat{t}_v \in \mathbb{R}^n, \quad \|K_v^{-1/2}\hat{t}_v\| \leq 1\} \quad \text{if } \theta_v = 0.$$

Let $\hat{\theta}_v$ be the minimizer of $C_{g,v}$. The sub-differential equations above give the two following cases:

Case 1. If $\hat{\theta}_v = 0$ then there exists $\hat{t}_v \in \mathbb{R}^n$ such that $\|K_v^{-1/2}\hat{t}_v\| \leq 1$ and it fulfils Equation (17):

$$2K_vR_v = \sqrt{n}\mu_g\hat{t}_v,$$

So, the necessary and sufficient condition for which the solution $\hat{\theta}_v = 0$ is the optimal one is:

$$\left\| \frac{2}{\sqrt{n}}K_v^{1/2}R_v \right\| \leq \mu_g.$$

Case 2. If $\hat{\theta}_v \neq 0$ then $\hat{t}_v = K_v\hat{\theta}_v/\|K_v^{1/2}\hat{\theta}_v\|$ and it fulfils Equation (17):

$$2K_v(R_v - K_v\hat{\theta}_v) = \sqrt{n}\mu_g \frac{K_v\hat{\theta}_v}{\|K_v^{1/2}\hat{\theta}_v\|}.$$

We obtain then,

$$\hat{\theta}_v = \left(K_v + \frac{\sqrt{n}\mu_g}{2\|K_v^{1/2}\hat{\theta}_v\|} I_n \right)^{-1} R_v. \quad (18)$$

Since $\hat{\theta}_v$ appears in both sides of the Equation (18), a numerical procedure is needed:

Proposition A.1 For $\rho > 0$ let $\theta(\rho) = (K_v + \rho I_n)^{-1} R_v$. There exists a non zero solution to Equation (18) if and only if there exists $\rho > 0$ such that

$$\mu_g = \frac{2\rho}{\sqrt{n}} \|K_v^{1/2}\theta(\rho)\|. \quad (19)$$

Then $\hat{\theta}_v = \theta(\rho)$.

Proof If there exists a non zero solution to Equation (18), then $\|K_v^{1/2}\hat{\theta}_v\| \neq 0$ since K_v is positive definite. Take

$$\rho = \frac{\sqrt{n}\mu_g}{2\|K_v^{1/2}\hat{\theta}_v\|},$$

then

$$\theta(\rho) = (K_v + \frac{\sqrt{n}\mu_g}{2\|K_v^{1/2}\hat{\theta}_v\|}I_n)^{-1}R_v = \hat{\theta}_v,$$

and, for such ρ Equation (19) is satisfied.

Conversely, if there exists $\rho > 0$ such that Equation (19) is satisfied, then $\|K_v^{1/2}\theta(\rho)\| \neq 0$ and,

$$\rho = \frac{\sqrt{n}\mu_g}{2\|K_v^{1/2}\theta(\rho)\|}.$$

Therefore,

$$\theta(\rho) = (K_v + \frac{\sqrt{n}\mu_g}{2\|K_v^{1/2}\theta(\rho)\|}I_n)^{-1}R_v,$$

which is Equation (18) calculated in $\hat{\theta}_v = \theta(\rho)$. \square

Remark A.1 Define $y(\rho) = 2\rho\|K_v^{1/2}\theta(\rho)\| - \sqrt{n}\mu_g$ with $\theta(\rho) = (K_v + \rho I_n)^{-1}R_v$, then $y(\rho) = 0$ has a unique solution, denoted $\hat{\rho}$, which leads to calculate $\hat{\theta}(\hat{\rho})$.

Proof For $\rho = 0$ we have $y(0) = -\sqrt{n}\mu_g < 0$, since $\mu_g > 0$; and for $\rho \rightarrow +\infty$ we have $y(\rho) > 0$, since $\|K_v^{1/2}(\frac{K_v}{\rho} + I_n)^{-1}R_v\| \rightarrow \|K_v^{1/2}R_v\|$ and $\|2K_v^{1/2}R_v\| > \sqrt{n}\mu_g$.

Moreover, we have

$$\begin{aligned} y(\rho) &= 2\|(\frac{I_n}{\rho} + k_v^{-1})^{-1}k_v^{-1/2}R_v\| - \sqrt{n}\mu_g, \\ &= 2(X^T A^{-2}X)^{1/2} - \sqrt{n}\mu_g, \end{aligned}$$

where $A = (I_n/\rho + k_v^{-1})$ and $X = k_v^{-1/2}R_v$. The first derivative of $y(\rho)$ in ρ is obtained by,

$$\frac{\partial y(\rho)}{\partial \rho} = (X^T A^{-2}X)^{-1/2} \frac{\partial (X^T A^{-2}X)}{\partial \rho},$$

and,

$$\begin{aligned} \frac{\partial (X^T A^{-2}X)}{\partial \rho} &= X^T \frac{\partial (A^{-1})^2}{\partial \rho} X, \\ &= 2X^T A^{-1}(-A^{-1} \frac{\partial A}{\partial \rho} A^{-1})X, \\ &= \frac{2}{\rho^2} \|A^{-3/2}X\|. \end{aligned}$$

Finally, we get

$$\frac{\partial y(\rho)}{\partial \rho} = \frac{2\|(\frac{I_n}{\rho} + k_v^{-1})^{-3/2}k_v^{-1/2}R_v\|}{\rho^2\|(\frac{I_n}{\rho} + k_v^{-1})^{-1}k_v^{-1/2}R_v\|} > 0.$$

So $y(\rho)$ is an increasing function of ρ , and the proof is complete. \square

Algorithm 4 Algorithm to find ρ as well as $\hat{\theta}_v$

```

1: if  $\hat{\theta}_{\text{old}} = 0$  then      ▷  $\hat{\theta}_{\text{old}}$  is  $\hat{\theta}_v$  computed in the previous step of the RKHS group lasso
   algorithm.
2:   Set  $\rho \leftarrow 1$  and calculate  $y(\rho)$ 
3:   if  $y(\rho) > 0$  then
4:     Find  $\hat{\rho}$  that minimizes  $y(\rho)$  on the interval  $[0, 1]$ 
5:   else
6:     repeat
7:       Set  $\rho \leftarrow \rho \times 10$  and calculate  $y(\rho)$ 
8:     until  $y(\rho) > 0$ 
9:     Find  $\hat{\rho}$  that minimizes  $y(\rho)$  on the interval  $[\rho/10, \rho]$ 
10:  end if
11: else
12:  Set  $\rho \leftarrow \frac{\sqrt{n}\mu_g}{2\|K_v^{1/2}\hat{\theta}_{\text{old}}\|}$  and calculate  $y(\rho)$ 
13:  if  $y(\rho) > 0$  then
14:    repeat
15:      Set  $\rho \leftarrow \rho/10$  and calculate  $y(\rho)$ 
16:    until  $y(\rho) < 0$ 
17:    Find  $\hat{\rho}$  that minimizes  $y(\rho)$  on the interval  $[\rho, \rho \times 10]$ 
18:  else
19:    repeat
20:      Set  $\rho \leftarrow \rho \times 10$  and calculate  $y(\rho)$ 
21:    until  $y(\rho) > 0$ 
22:    Find  $\hat{\rho}$  that minimizes  $y(\rho)$  on the interval  $[\rho/10, \rho]$ 
23:  end if
24: end if
25: calculate  $\hat{\theta}_v = \theta(\hat{\rho})$ 

```

In order to calculate ρ and so $\hat{\theta}_v = \theta(\rho)$ we use Algorithm 4 which is a part of the RKHS group lasso Algorithm 1 when $\hat{\theta}_v \neq 0$.

RKHS ridge group sparse algorithm

We consider the minimization of the RKHS ridge group sparse criteria:

$$C(f_0, \theta) = \|Y - f_0 I_n - \sum_{v \in \mathcal{P}} K_v \theta_v\|^2 + \sqrt{n}\gamma \sum_{v \in \mathcal{P}} \|K_v \theta_v\| + n\mu \sum_{v \in \mathcal{P}} \|K_v^{1/2} \theta_v\|.$$

The constant term f_0 is estimated as in the RKHS group lasso algorithm. In order to calculate $\hat{\theta} = \operatorname{argmin}_{\theta \in \mathbb{R}^{n \times |\mathcal{P}|}} C(f_0, \theta)$, we use once again the block coordinate descent algorithm group v by group v . In the following, we fix a group v , and we find the minimizer of $C(f_0, \theta)$ with respect to θ_v for given values of f_0 and θ_w , $w \neq v$. We aim at minimizing with respect to θ_v ,

$$C_v(f_0, \theta_v) = \|R_v - K_v \theta_v\|^2 + \sqrt{n}\gamma \|K_v \theta_v\| + n\mu \|K_v^{1/2} \theta_v\|,$$

where R_v is defined by (16).

Let ∂C_v be the sub-differential of $C_v(f_0, \theta_v)$ with respect to θ_v ,

$$\partial C_v = \{-2K_v(R_v - K_v \theta_v) + \sqrt{n}\gamma s_v + n\mu t_v \quad : \quad s_v \in \partial \|K_v \theta_v\|, \quad t_v \in \partial \|K_v^{1/2} \theta_v\|\},$$

According to the first order optimality condition (see Preliminary A.2), we know that there exists $\hat{s}_v \in \partial\|K_v\theta_v\|$ and $\hat{t}_v \in \partial\|K_v^{1/2}\theta_v\|$ such that,

$$-2K_v(R_v - K_v\theta_v) + \sqrt{n}\gamma\hat{s}_v + n\mu\hat{t}_v = 0. \quad (20)$$

The sub-differential definition (see Preliminary A.1) gives,

$$\{\partial\|K_v^{1/2}\theta_v\| = \left\{ \frac{K_v\theta_v}{\|K_v^{1/2}\theta_v\|} \right\}, \quad \partial\|K_v\theta_v\| = \left\{ \frac{K_v^2\theta_v}{\|K_v\theta_v\|} \right\}\} \quad \text{if } \theta_v \neq 0,$$

and,

$$\{\partial\|K_v^{1/2}\theta_v\| = \{\hat{t}_v \in \mathbb{R}^n, \|K_v^{-1/2}\hat{t}_v\| \leq 1\}, \quad \partial\|K_v\theta_v\| = \{\hat{s}_v \in \mathbb{R}^n, \|K_v^{-1}\hat{s}_v\| \leq 1\}\} \quad \text{if } \theta_v = 0.$$

Let $\hat{\theta}_v$ be the minimizer of the $C_v(f_0, \theta_v)$. Using the sub-differential equations above, the estimator $\hat{\theta}_v$, $v \in \mathcal{P}$ is obtained following two cases below:

Case 1. If $\hat{\theta}_v = 0$ then there exists $\hat{s}_v \in \mathbb{R}^n$ such that $\|K_v^{-1}\hat{s}_v\| \leq 1$ and it fulfils Equation (20):

$$2K_vR_v - n\mu\hat{t}_v = \sqrt{n}\gamma\hat{s}_v,$$

with $\hat{t}_v \in \mathbb{R}^n$, $\|K_v^{-1/2}\hat{t}_v\| \leq 1$. Set

$$J(\hat{t}_v) = \|2R_v - n\mu K_v^{-1}\hat{t}_v\|,$$

and,

$$J^* = \operatorname{argmin}_{\hat{t}_v \in \mathbb{R}^n} \{J(\hat{t}_v), \text{ such that } \|K_v^{-1/2}\hat{t}_v\| \leq 1\}.$$

Then the solution to Equation (20) is zero if and only if $J^* \leq \gamma$.

Case 2. If $\hat{\theta}_v \neq 0$ then we have $\hat{s}_v = K_v^2\hat{\theta}_v/\|K_v\hat{\theta}_v\|$, and $\hat{t}_v = K_v\hat{\theta}_v/\|K_v^{1/2}\hat{\theta}_v\|$ fulfilling Equation (20):

$$2K_v(R_v - K_v\hat{\theta}_v) = \sqrt{n}\gamma \frac{K_v^2\hat{\theta}_v}{\|K_v\hat{\theta}_v\|_2} + n\mu \frac{K_v\hat{\theta}_v}{\|K_v^{1/2}\hat{\theta}_v\|},$$

that is,

$$\hat{\theta}_v = (K_v + \frac{\sqrt{n}\gamma}{2\|K_v\hat{\theta}_v\|}K_v + \frac{n\mu}{2\|K_v^{1/2}\hat{\theta}_v\|}I_n)^{-1}R_v \quad \text{if } \hat{\theta}_v \neq 0.$$

In this case the calculation of $\hat{\theta}_v$ needs a numerical algorithm which is explained in [Huet and Taupin \(2017\)](#).

Affiliation:

Halaleh Kamari

Laboratoire LaMME, UMR CNRS 8071- USC INRA, Université d'Évry Val d'Essonne, France

UR 1404 MaIAGE, INRA Jouy-en-Josas, France

E-mail: halaleh.kamari@univ-evry.fr

URL: <http://www.math-evry.cnrs.fr/members/hkamari/welcome>

Sylvie Huet

UR 1404 MaIAGE, INRA Jouy-en-Josas, France

E-mail: shuet.inra@gmail.com

URL: <http://genome.jouy.inra.fr/~shuet/>

Marie-Luce Taupin

Laboratoire LaMME, UMR CNRS 8071- USC INRA, Université d'Évry Val d'Essonne, France

E-mail: marie-luce.taupin@univ-evry.fr

URL: <http://www.math-evry.cnrs.fr/members/mtaupin/welcome>