

Package ‘RKHSMetaMod’

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Type Package

Title Ridge Group Sparse Optimization Problem for Estimation of a Meta Model Based on Reproducing Kernel Hilbert Spaces

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Description

Estimates the Hoeffding decomposition of an unknown function by solving ridge group sparse optimization problem based on reproducing kernel Hilbert spaces, and approximates its sensitivity indices (see Kamari, H., Huet, S. and Taupin, M.-L. (2019) <arXiv:1905.13695>).

License GPL (>= 2)

Imports Rcpp (>= 1.0.0)

Suggests lhs

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RKHSMetaMod-package	<i>Set of Rcpp and R functions to produce a sequence of meta models that are the solutions of the RKHS Ridge Group Sparse or RKHS Group Lasso optimization problems, calculate their associated prediction errors as well as their empirical sensitivity indices.</i>
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Description

Fits a meta model to an unknown model m by solving the ridge group sparse (or group lasso) optimization problem based on the reproducing kernel Hilbert spaces (RKHS), for the Gaussian regression model :

$$Y = m(X) + \sigma\varepsilon,$$

where variables X_1, \dots, X_d are independent and uniformly distributed on $[0, 1]$ and are independent of ε 's.

We define the ridge group sparse criteria by :

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

and the group lasso criteria is obtained by setting $\gamma = 0$ in the criteria above. We set $\mu_g = \sqrt{n} \mu$ to be the group lasso penalty parameter.

For each pair of the penalty parameters (μ, γ) in the ridge group sparse criteria, one meta model, called RKHS meta model, is calculated. The RKHS meta model is an additive model with at most $vMax$ groups. It satisfies the properties of the Hoeffding decomposition, and its terms estimate the terms in the Hoeffding decomposition of the function m .

These estimators are evaluated using a testing dataset. That is, the prediction error is calculated for each RKHS meta model and the one with the minimum prediction error is the "best" estimator for the true model m . It provides a function that estimates the empirical sensitivity indices of the "best" RKHS meta model as an approximation of the true sensitivity indices.

Details

Details.

Author(s)

Halaleh Kamari.

Maintainer: <halaleh.kamari@univ-evry.fr>

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoeffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also[RKHSMetaMod](#)**Examples**

```

d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2,0.6,0.8)
F <- 1;for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n,0,1);sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
frc <- c(10,100)
gamma <- c(.5,.01,.001,0)
result <- RKHSMetMod(Y,X,kernel,Dmax,gamma,frc,FALSE)

```

calc_Kv

Function to calculate the Gram matrices and their eigenvalues and eigenvectors for a chosen reproducing kernel.

Description

Calculates the Gram matrices K_v for $v = 1, \dots, vMax$, and returns their associated eigenvalues and eigenvectors. The calculated Gram matrices may be not positive definite. The option "correction" of this function allows to replace the matrices K_v that are not positive definite by their "nearest positive definite" matrices.

Usage

```
calc_Kv(X, kernel, Dmax, correction, verbose, tol)
```

Arguments

X	Matrix of observations with n rows and d columns.
kernel	Character, the type of the reproducing kernel: matern (matern kernel), brownian (brownian kernel), gaussian (gaussian kernel), linear (linear kernel), quad (quadratic kernel).
Dmax	Integer, between 1 and d , indicates the order of interactions considered in the meta model: Dmax= 1 is used to consider only the main effects, Dmax= 2 to include the main effects and the interactions of order 2, . . .
correction	Logical, if TRUE, the program makes the correction to the matrices K_v that are not positive definite (see details). Set as TRUE by default.
verbose	Logical, if TRUE, the group v for which the correction is done is printed. Set as TRUE by default.

tol Scalar, used if correction is TRUE. For each matrix K_v if $\lambda_{min} < \lambda_{max} \times tol$, then the correction to K_v is done (see details). Set as $1e^{-8}$ by default.

Details

Let $\lambda_{v,i}, i = 1, \dots, n$ be the eigenvalues associated with matrix K_v . Set $\lambda_{max} = \max_i \lambda_{v,i}$ and $\lambda_{min} = \min_i \lambda_{v,i}$. The eigenvalues of K_v that is not positive definite are replaced by $\lambda_{v,i} + \epsilon$, with $\epsilon = \lambda_{max} \times tol$. The value of tol depends on the type of the kernel and it is chosen small.

Value

List of two components "names.Grp" and "kv":

names.Grp	Vector of size vMax, indicates the name of groups included in the meta model.
kv	List of vMax components with the same names as the vector names.Grp. Each element of the list is a list of two components "Evalues" and "Q":
Evalues	Vector of size n , eigenvalues of each Gram matrix K_v .
Q	Matrix with n rows and n columns, eigenvectors of each Gram matrix K_v .

Note

Note.

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

[RKHSMetaMod](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n, 0, 1); sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
Kv <- calc_Kv(X, kernel, Dmax)
```

```
names <- Kv$names.Grp
Eigen.val1 <- Kv$kv$v1.$Evalues
Eigen.vec1 <- Kv$kv$v1.$Q
```

grplasso_q	<i>Function to fit a solution with q active groups of an RKHS Group Lasso problem.</i>
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Description

Fits a solution of the group lasso problem based on RKHS, with q active groups in the obtained solution for the Gaussian regression model. It determines $\mu_g(q)$, for which the number of active groups in the solution of the RKHS group lasso problem is equal to q , and returns the RKHS meta model associated with $\mu_g(q)$.

Usage

```
grplasso_q(Y, Kv, q, rat, Num)
```

Arguments

Y	Vector of response observations of size n .
Kv	List of eigenvalues and eigenvectors of positive definite Gram matrices K_v and their associated group names. It should have the same format as the output of the function <code>calc_Kv</code> (see details).
q	Integer, the number of active groups in the obtained solution.
rat	Positive scalar, used to restrict the minimum value of μ_g , to be evaluated in the RKHS Group Lasso algorithm, $\mu_{min} = \mu_{max}/rat$. The value μ_{max} is calculated inside the program, see function <code>mu_max</code> .
Num	Integer, used to restrict the number of different values of the penalty parameter μ_g to be evaluated in the RKHS Group Lasso algorithm, until it achieves $\mu_g(q)$: for Num = 1 the program is done for 3 values of μ_g , $\mu_1 = (\mu_{min} + \mu_{max})/2$, $\mu_2 = (\mu_{min} + \mu_1)/2$ or $\mu_2 = (\mu_1 + \mu_{max})/2$ depending on the value of q associated with $\mu_1, \mu_3 = \mu_{min}$.

Details

Input Kv should contain the eigenvalues and eigenvectors of positive definite Gram matrices K_v . It is necessary to set input "correction" in the function `calc_Kv` equal to "TRUE".

Value

List of 4 components: "mus", "qs", "mu", "res":

mus	Vector, values of the evaluated penalty parameters μ_g in the RKHS group lasso algorithm until it achieves $\mu_g(q)$.
qs	Vector, number of active groups associated with each value of μ_g in mus.

mu	Scalar, value of $\mu_g(q)$.
res	An RKHS Group Lasso object:
intercept	Scalar, estimated value of intercept.
teta	Matrix with vMax rows and n columns. Each row of the matrix is the estimated vector θ_v for $v = 1, \dots, vMax$.
fit.v	Matrix with n rows and vMax columns. Each row of the matrix is the estimated value of $f_v = K_v \theta_v$.
fitted	Vector of size n , indicates the estimator of m .
Norm.H	Vector of size vMax, estimated values of the penalty norm.
supp	Vector of active groups.
Nsupp	Vector of the names of the active groups.
SCR	Scalar, equals to $\ Y - f_0 - \sum_v K_v \theta_v\ ^2$.
crit	Scalar, indicates the value of the penalized criteria.
MaxIter	Integer, number of iterations until convergence is reached.
convergence	TRUE or FALSE. Indicates whether the algorithm has converged or not.
RelDiffCrit	Scalar, value of the first convergence criteria at the last iteration, $\frac{crit_{lastIter} - crit_{lastIter-1}}{crit_{lastIter-1}}$.
RelDiffPar	Scalar, value of the second convergence criteria at the last iteration, $\ \frac{\theta_{lastIter} - \theta_{lastIter-1}}{\theta_{lastIter-1}}\ ^2$.

Note

Note.

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

[calc_Kv](#), [mu_max](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n,0,1); sigma <- 0.2
```

```
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
Kv <- calc_Kv(X, kernel, Dmax, TRUE, TRUE)
result <- grplasso_q(Y,Kv,5,100 ,Num=10)
result$mu
result$res$Nsupp
```

mu_max	<i>Function to find the maximal value of the penalty parameter in the RKHS Group Lasso problem.</i>
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Description

Calculates the value of the penalty parameter in the RKHS group lasso problem when the first penalized parameter group enters the model.

Usage

```
mu_max(Y, matZ)
```

Arguments

Y	Vector of response observations of size n .
matZ	List of vMax components. Each component includes the eigenvalues and eigenvectors of the positive definite Gram matrices $K_v, v = 1, \dots, vMax$. It should have the same format as the output "kv" of the function calc_Kv .

Details

Details.

Value

An object of type numeric is returned.

Note

Note.

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

Meier, L. Van de Geer, S. and Buhlmann, P. (2008) The group LASSO for logistic regression. Journal of the Royal Statistical Society Series B. 70. 53-71. 10.1111/j.1467-9868.2007.00627.x.

See Also

[calc_Kv](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2,0.6,0.8)
F <- 1;for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n,0,1);sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
Kv <- calc_Kv(X, kernel, Dmax, TRUE,TRUE)
matZ <- Kv$kv
mumax <- mu_max(Y, matZ)
mumax
```

pen_MetMod

Function to fit a solution of the RKHS Ridge Group Sparse problem.

Description

Fits the solution of the RKHS ridge group sparse optimization problem for the Gaussian regression model.

Usage

```
pen_MetMod(Y, Kv, gamma, mu, resg, gama_v, mu_v, maxIter, verbose, calcStwo)
```

Arguments

Y	Vector of response observations of size n .
Kv	List, includes the eigenvalues and eigenvectors of the positive definite Gram matrices $K_v, v = 1, \dots, vMax$ and their associated group names. It should have the same format as the output of the function calc_Kv (see details).
gamma	Vector of positive scalars. Values of the penalty parameter γ in decreasing order.

mu	Vector of positive scalars. Values of the penalty parameter μ in decreasing order.
resg	List of initial parameters, includes the <code>RKHSgrplasso</code> objects for each value of the penalty parameter μ .
gama_v	Scalar zero or vector of vMax positive scalars, considered as weights for the Ridge penalty. Set to zero, to consider no weights, i.e. all weights equal to 1.
mu_v	Scalar zero or a vector with vMax scalars, considered as weights of Sparse Group penalty. Set to zero, to consider no weights, i.e. all weights equal to 1.
maxIter	Integer, shows the maximum number of loops through initial active groups at the first step and maximum number of loops through all groups at the second step. Set as 1000 by default.
verbose	Logical, if TRUE, for each pair of penalty parameters (μ, γ) it prints: the number of current iteration, active groups and convergence criterias. Set as FALSE by default.
calcStwo	Logical, if TRUE, the program does a second step after convergence: the algorithm is done over all groups by taking the estimated parameters at the first step as initial values. Set as FALSE by default.

Details

Input `Kv` should contain the eigenvalues and eigenvectors of positive definite Gram matrices K_v . It is necessary to set input "correction" in the function `calc_Kv` equal to "TRUE".

Value

List of `l` components, with `l` equals to the number of pairs of the penalty parameters (μ, γ) . Each component of the list is a list of 3 components "mu", "gamma" and "Meta-Model":

mu	Positive scalar, an element of the input vector mu associated with the estimated Meta-Model.
gamma	Positive scalar, an element of the input vector gamma associated with the estimated Meta-Model.
Meta-Model	Estimated meta model associated with penalty parameters mu and gamma. List of 16 components:
intercept	Scalar, estimated value of intercept.
teta	Matrix with vMax rows and n columns. Each row of the matrix is the estimated vector θ_v for $v = 1, \dots, vMax$.
fit.v	Matrix with n rows and vMax columns. Each row of the matrix is the estimated value of $f_v = K_v \theta_v$.
fitted	Vector of size n , indicates the estimator of m .
Norm.n	Vector of size vMax, estimated values for the Ridge penalty norm.
Norm.H	Vector of size vMax, estimated values for the Group Sparse penalty norm.
supp	Vector of active groups.
Nsupp	Vector of the names of the active groups.

SCR	Scalar equals to $\ Y - f_0 - \sum_v K_v \theta_v\ ^2$.
crit	Scalar indicates the value of the penalized criteria.
gamma.v	Vector of size vMax, coefficients of the Ridge penalty norm, $\sqrt{n}\gamma \times \text{gama}_v$.
mu.v	Vector of size vMax, coefficients of the Group Sparse penalty norm, $n\mu \times \text{mu}_v$.
iter	List of three components if calcStwo=TRUE (two components if calcStwo=FALSE): maxIter, number of iterations until convergence is reached at first step and the number of iterations until convergence is reached at second step (maxIter, and the number of iterations until convergence is reached at first step).
convergence	TRUE or FALSE. Indicates whether the algorithm has converged or not.
RelDiffCrit	List of two components if calcStwo=TRUE (one component if calcStwo=FALSE): value of convergence criteria at the last iteration of each step, $\left\ \frac{\theta_{lastIter} - \theta_{lastIter-1}}{\theta_{lastIter-1}} \right\ ^2$.
RelDiffPar	List of two components if calcStwo=TRUE (one component if calcStwo=FALSE): value of convergence criteria at the last iteration, $\frac{crit_{lastIter} - crit_{lastIter-1}}{crit_{lastIter-1}}$ of each step.

Note

Note.

Author(s)

Halaleh Kamari

References

Huet, S. and Taupin, M. L. (2017) Metamodel construction for sensitivity analysis. *ESAIM: Proc* 60, 27-69.

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

[calc_Kv](#), [RKHSgrplasso](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n, 0, 1); sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
Kv <- calc_Kv(X, kernel, Dmax, TRUE, TRUE, tol = 1e-08)
```

```

vMax <- length(Kv$names.Grp)
matZ <- Kv$kv
mumax <- mu_max(Y, matZ)
mug1 <- mumax/10
mug2 <- mumax/100
gr1 <- RKHSgrplasso(Y,Kv, mug1)
gr2 <- RKHSgrplasso(Y,Kv, mug2)
gamma <- c(.5,.01,.001)
#rescaling the penalty parameter
mu <- c(mug1/sqrt(n),mug2/sqrt(n))
resg <- list(gr1,gr2)
res <- pen_MetMod(Y,Kv,gamma,mu,resg,0,0)
l <- length(res)
for(i in 1:l){print(res[[i]]$mu)}
for(i in 1:l){print(res[[i]]$gamma)}
for(i in 1:l){print(res[[i]]$`Meta-Model`$Nsupp)}
gama_v <- rep(1,vMax)
mu_v <- rep(1,vMax)
res.w <- pen_MetMod(Y,Kv,gamma,mu,resg,gama_v,mu_v)
for(i in 1:l){print(res.w[[i]]$`Meta-Model`$Nsupp)}

```

PredErr

Function to calculate the prediction error.

Description

Computes the prediction error by considering a testing dataset.

Usage

```
PredErr(X, XT, YT, mu, gamma, res, kernel, Dmax)
```

Arguments

X	Matrix of observations with n rows and d columns.
XT	Matrix of observations of the testing dataset with n^{test} rows and d columns.
YT	Vector of response observations of testing dataset of size n^{test} .
mu	Vector of positive scalars. Values of the Group Sparse penalty parameter in decreasing order. See function RKHSMetMod .
gamma	Vector of positive scalars. Values of the Ridge penalty parameter in decreasing order. See function RKHSMetMod .
res	List, includes a sequence of estimated meta models for the learning dataset, using RKHS Ridge Group Sparse or RKHS Group Lasso algorithm, associated with the penalty parameters mu and gamma. It should have the same format as the output of one of the functions: pen_MetMod , RKHSMetMod or RKHSMetMod_qmax .
kernel	Character, shows the type of the reproducing kernel: matern, brownian, gaussian, linear, quad. The same kernel should be chosen as the one used for the learning dataset. See function calc_Kv .

Dmax Integer between 1 and d . The same Dmax should be chosen as the one used for learning dataset. See function `calc_Kv`.

Details

Details.

Value

Matrix of the prediction errors is returned. Each element of the matrix is the obtained prediction error associated with one RKHS meta model in "res".

Note

Note.

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

`calc_Kv`, `pen_MetMod`, `RKHSMetMod`, `RKHSMetMod_qmax`

Examples

```
d <- 3
n <- 50
nT <- 50
library(lhs)
X <- maximinLHS(n, d)
XT <- maximinLHS(nT, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
FT <- 1; for (a in 1:d) FT <- FT*(abs(4*XT[,a]-2)+c[a])/(1+c[a])
sigma <- 0.2
epsilon <- rnorm(n, 0, 1); Y <- F + sigma*epsilon
epsilonT <- rnorm(nT, 0, 1); YT <- FT + sigma*epsilonT
Dmax <- 3
kernel <- "matern"
frc <- c(10, 100)
gamma <- c(.5, .01, .001)
res <- RKHSMetMod(Y, X, kernel, Dmax, gamma, frc, FALSE)
mu <- vector()
l <- length(gamma)
for(i in 1:length(frc)){mu[i]=res[[(i-1)*1+1]]$mu}
```

```
error <- PredErr(X,XT, YT,mu,gamma, res, kernel,Dmax)
error
```

 RKHSgrplasso

Function to fit a solution of an RKHS Group Lasso problem.

Description

Fits the solution of an RKHS group lasso problem for the Gaussian regression model.

Usage

```
RKHSgrplasso(Y, Kv, mu, maxIter, verbose)
```

Arguments

Y	Vector of response observations of size n .
Kv	List, includes the eigenvalues and eigenvectors of the positive definite Gram matrices $K_v, v = 1, \dots, vMax$ and their associated group names. It should have the same format as the output of the function calc_Kv (see details).
mu	Positive scalar, value of the penalty parameter μ_g in the RKHS Group Lasso problem.
maxIter	Integer, shows the maximum number of loops through all groups. Set as 1000 by default.
verbose	Logical, if TRUE, prints: the number of current iteration, active groups and convergence criterias. Set as FALSE by default.

Details

Input Kv should contain the eigenvalues and eigenvectors of positive definite Gram matrices K_v . It is necessary to set input correction in the function [calc_Kv](#) equal to "TRUE".

Value

Estimated RKHS meta model, list with 13 components:

intercept	Scalar, estimated value of intercept.
teta	Matrix with vMax rows and n columns. Each row of the matrix is the estimated vector θ_v for $v = 1, \dots, vMax$.
fit.v	Matrix with n rows and vMax columns. Each row of the matrix is the estimated value of $f_v = K_v \theta_v$.
fitted	Vector of size n , indicates the estimator of m .
Norm.H	Vector of size vMax, estimated values of the penalty norm.
supp	Vector of active groups.
Nsupp	Vector of the names of the active groups.

SCR	Scalar, equals to $\ Y - f_0 - \sum_v K_v \theta_v\ ^2$.
crit	Scalar, indicates the value of penalized criteria.
MaxIter	Integer, number of iterations until convergence is reached.
convergence	TRUE or FALSE. Indicates whether the algorithm has converged or not.
RelDiffCrit	Scalar, value of the first convergence criteria at the last iteration, $\frac{crit_{lastIter} - crit_{lastIter-1}}{crit_{lastIter-1}}$.
RelDiffPar	Scalar, value of the second convergence criteria at the last iteration, $\left\ \frac{\theta_{lastIter} - \theta_{lastIter-1}}{\theta_{lastIter-1}} \right\ ^2$.

Note

Note.

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

Meier, L. Van de Geer, S. and Bühlmann, P. (2008) The group LASSO for logistic regression. Journal of the Royal Statistical Society Series B. 70. 53-71. 10.1111/j.1467-9868.2007.00627.x.

See Also

[calc_Kv](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n, 0, 1); sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
Kv <- calc_Kv(X, kernel, Dmax, TRUE, TRUE)
matZ <- Kv$kv
mumax <- mu_max(Y, matZ)
mug <- mumax/10
gr <- RKHSgrplasso(Y, Kv, mug, 1000, FALSE)
gr$Nsupp
```

RKHSMetMod	<i>Function to produce a sequence of meta models that are the solutions of the RKHS Ridge Group Sparse or RKHS Group Lasso optimization problems.</i>
------------	---

Description

Calculates the Gram matrices K_v for a chosen reproducing kernel and fits the solution of an RKHS ridge group sparse or an RKHS group lasso problem for each pair of penalty parameters (μ, γ) , for the Gaussian regression model.

Usage

```
RKHSMetMod(Y, X, kernel, Dmax, gamma, frc, verbose)
```

Arguments

Y	Vector of response observations of size n .
X	Matrix of observations with n rows and d columns.
kernel	Character, indicates the type of the reproducing kernel: matern (matern kernel), brownian (brownian kernel), gaussian (gaussian kernel), linear (linear kernel), quad (quadratic kernel). See the function calc_Kv
Dmax	Integer, between 1 and d , indicates the order of interactions considered in the meta model: Dmax= 1 is used to consider only the main effects, Dmax= 2 to include the main effects and the interactions of order 2, ... See the function calc_Kv
gamma	Vector of non negative scalars, values of the penalty parameter γ in decreasing order. If $\gamma = 0$ the function solves an RKHS Group Lasso problem and for $\gamma > 0$ it solves an RKHS Ridge Group Sparse problem.
frc	Vector of positive scalars. Each element of the vector sets a value to the penalty parameter μ , $\mu = \mu_{max}/(\sqrt{n} \times frc)$. The value μ_{max} is calculated by the program. See the function mu_max .
verbose	Logical, if TRUE, prints: the group v for which the correction of Gram matrix K_v is done, and for each pair of the penalty parameters (μ, γ) : the number of current iteration, active groups and convergence criterias. Set as FALSE by default.

Details

Details.

Value

List of l components, with l equals to the number of pairs of the penalty parameters (μ, γ) . Each component of the list is a list of 3 components "mu", "gamma" and "Meta-Model":

mu	Positive scalar, penalty parameter μ associated with the estimated Meta-Model.
gamma	Positive scalar, an element of the input vector gamma associated with the estimated Meta-Model.
Meta-Model	An RKHS Ridge Group Sparse or RKHS Group Lasso object associated with the penalty parameters mu and gamma:
intercept	Scalar, estimated value of intercept.
teta	Matrix with vMax rows and n columns. Each row of the matrix is the estimated vector θ_v for $v = 1, \dots, vMax$.
fit.v	Matrix with n rows and vMax columns. Each row of the matrix is the estimated value of $f_v = K_v \theta_v$.
fitted	Vector of size n , indicates the estimator of m .
Norm.n	Vector of size vMax, estimated values for the Ridge penalty norm.
Norm.H	Vector of size vMax, estimated values of the Sparse Group penalty norm.
supp	Vector of active groups.
Nsupp	Vector of the names of the active groups.
SCR	Scalar, equals to $\ Y - f_0 - \sum_v K_v \theta_v\ ^2$.
crit	Scalar, indicates the value of the penalized criteria.
gamma.v	Vector of size vMax, coefficients of the Ridge penalty norm, $\sqrt{n}\gamma \times \text{gama}_v$.
mu.v	Vector of size vMax, coefficients of the Group Sparse penalty norm, $n\mu \times \text{mu}_v$.
iter	List of two components: maxIter, and the number of iterations until the convergence is achieved.
convergence	TRUE or FALSE. Indicates whether the algorithm has converged or not.
RelDiffCrit	Scalar, value of the first convergence criteria at the last iteration, $\ \frac{\theta_{lastIter} - \theta_{lastIter-1}}{\theta_{lastIter-1}}\ ^2$.
RelDiffPar	Scalar, value of the second convergence criteria at the last iteration, $\frac{crit_{lastIter} - crit_{lastIter-1}}{crit_{lastIter-1}}$.

Note

For the case $\gamma = 0$ the outputs "mu" = μ_g and "Meta-Model" is the same as the one returned by the function [RKHSgrplasso](#).

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

[calc_Kv](#), [mu_max](#), [RKHSgrplasso](#), [pen_MetMod](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n,0,1); sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
frc <- c(10,100)
gamma <- c(.5, .01, .001, 0)
result <- RKHSMetMod(Y, X, kernel, Dmax, gamma, frc, FALSE)
l <- length(result)
for(i in 1:l){print(result[[i]]$mu)}
for(i in 1:l){print(result[[i]]$gamma)}
for(i in 1:l){print(result[[i]]$`Meta-Model`$Nsupp)}
```

RKHSMetMod_qmax

Function to produce a sequence of meta models, with at most qmax active groups in each meta model. The meta models are the solutions of the RKHS Ridge Group Sparse or RKHS Group Lasso optimization problems.

Description

Calculates the Gram matrices K_v for a chosen kernel, determines μ , note $\mu(qmax)$, for which the number of active groups in the RKHS group lasso solution is equal to qmax, and fits a solution of an RKHS ridge group sparse or an RKHS group lasso problem for each pair of penalty parameters $(\mu(qmax), \gamma)$, in the Gaussian regression model.

Usage

```
RKHSMetMod_qmax(Y, X, kernel, Dmax, gamma, qmax, rat, Num, verbose)
```

Arguments

Y	Vector of response observations of size n .
X	Matrix of observations with n rows and d columns.
kernel	Character, indicates the type of the reproducing kernel: matern (matern kernel), brownian (brownian kernel), gaussian (gaussian kernel), linear (linear kernel), quad (quadratic kernel). See the function calc_Kv .

Dmax	Integer, between 1 and d , indicates the order of interactions considered in the meta model: Dmax= 1 is used to consider only the main effects, Dmax= 2 to include the main effects and the interactions of order 2, ... See the function <code>calc_Kv</code> .
gamma	Vector of non negative scalars, values of the penalty parameter γ in decreasing order. If $\gamma = 0$ the function solves an RKHS Group Lasso problem and for $\gamma > 0$ it solves an RKHS Ridge Group Sparse problem.
qmax	Integer, shows the maximum number of active groups in the obtained solution.
rat	Positive scalar, to restrict the minimum value of μ considered in the algorithm, $\mu_{min} = \mu_{max}/(\sqrt{n} \times rat)$. The value μ_{max} is calculated inside the program, see function <code>mu_max</code> .
Num	Integer, it is used to restrict the number of different values of the penalty parameter μ to be evaluated in the RKHS Group Lasso algorithm until it achieves $\mu(qmax)$: for Num = 1 the program is done for 3 different values of μ , $\mu_1 = (\mu_{min} + \mu_{max})/2$, $\mu_2 = (\mu_{min} + \mu_1)/2$ or $\mu_2 = (\mu_1 + \mu_{max})/2$ depending on the number of active groups in the meta model associated with μ_1 , $\mu_3 = \mu_{min}$.
verbose	Logical, if TRUE, prints: the group v for which the correction of Gram matrix K_v is done, and for each pair of (μ, γ) : the number of current iteration, active groups and convergence criterias. Set as FALSE by default.

Details

Details.

Value

List of three components "mus", "qs", and "MetaModel":

mus	Vector, values of the evaluated penalty parameters μ in the RKHS Group Lasso algorithm until it achieves $\mu(qmax)$.
qs	Vector, number of active groups associated with each element in mus.
MetaModel	List with the same length as the vector gamma. Each component of the list is a list of 3 components "mu", "gamma" and "Meta-Model":
mu	Scalar, the value $\mu(qmax)$.
gamma	Positive scalar, element of the input vector gamma associated with the estimated Meta-Model.
Meta-Model	An RKHS Ridge Group Sparse or RKHS Group Lasso object associated with the penalty parameters mu and gamma:
intercept	Scalar, estimated value of intercept.
teta	Matrix with vMax rows and n columns. Each row of the matrix is the estimated vector θ_v for $v = 1, \dots, vMax$.
fit.v	Matrix with n rows and vMax columns. Each row of the matrix is the estimated value of $f_v = K_v \theta_v$.
fitted	Vector of size n , indicates the estimator of m .
Norm.n	Vector of size vMax, estimated values for the Ridge penalty norm.

Norm.H	Vector of size vMax, estimated values of the Sparse Group penalty norm.
supp	Vector of active groups.
Nsupp	Vector of the names of the active groups.
SCR	Scalar, equals to $\ Y - f_0 - \sum_v K_v \theta_v\ ^2$.
crit	Scalar, indicates the value of penalized criteria.
gamma.v	Vector, coefficients of the Ridge penalty norm, $\sqrt{n}\gamma \times \text{gama}_v$.
mu.v	Vector, coefficients of the Group Sparse penalty norm, $n\mu \times \text{mu}_v$.
iter	List of two components: maxIter, and the number of iterations until the convergence is achieved.
convergence	TRUE or FALSE. Indicates whether the algorithm has converged or not.
RelDiffCrit	Scalar, value of the first convergence criteria at the last iteration, $\left\ \frac{\theta_{lastIter} - \theta_{lastIter-1}}{\theta_{lastIter-1}} \right\ ^2$.
RelDiffPar	Scalar, value of the second convergence criteria at the last iteration, $\frac{crit_{lastIter} - crit_{lastIter-1}}{crit_{lastIter-1}}$.

Note

For the case $\gamma = 0$ the outputs "mu" = μ_g and "Meta-Model" is the same as the one returned by the function [RKHSgrplasso](#).

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

[calc_Kv](#), [mu_max](#), [RKHSgrplasso](#), [pen_MetMod](#), [grplasso_q](#)

Examples

```
d <- 3
n <- 50
library(lhs)
X <- maximinLHS(n, d)
c <- c(0.2, 0.6, 0.8)
F <- 1; for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
epsilon <- rnorm(n, 0, 1); sigma <- 0.2
Y <- F + sigma*epsilon
Dmax <- 3
kernel <- "matern"
gamma <- c(.5, .01, .001, 0)
Num <- 10
rat <- 100
```

```

qmax <- 4
result <- RKHSMetMod_qmax(Y, X, kernel, Dmax, gamma, qmax, rat, Num, FALSE)
names(result)
result$mus
result$qss
l <- length(gamma)
for(i in 1:l){print(result$MetaModel[[i]]$mu)}
for(i in 1:l){print(result$MetaModel[[i]]$gamma)}
for(i in 1:l){print(result$MetaModel[[i]]$`Meta-Model`$Nsupp)}

```

SI_emp *Function to calculate the empirical sensitivity indices for an input or a group of inputs.*

Description

Calculates the empirical sensitivity indices.

Usage

```
SI_emp(res, ErrPred)
```

Arguments

res	List, includes a sequence of estimated meta models, the solutions of the RKHS Ridge Group Sparse or RKHS Group Lasso problems. It should have the same format as the output of one of the functions: pen_MetMod , RKHSMetMod or RKHSMetMod_qmax .
ErrPred	Matrix or NULL. If matrix, each element of the matrix is the obtained prediction error associated with one RKHS meta model in "res". It should have the same format as the output of the function PredErr . Set as "NULL" by default.

Details

Details.

Value

If input ErrPred≠"NULL", Vector of the empirical sensitivity indices for the meta model with the minimum Prediction error is returned. If ErrPred="NULL", a list of the vectors is returned. Each vector is the obtained sensitivity indices associated with one meta model in "res".

Note

Note.

Author(s)

Halaleh Kamari

References

Kamari, H., Huet, S. and Taupin, M.-L. (2019) RKHSMetaMod : An R package to estimate the Hoffding decomposition of an unknown function by solving RKHS Ridge Group Sparse optimization problem. <arXiv:1905.13695>

See Also

[PredErr](#), [pen_MetMod](#), [RKHSMetMod](#), [RKHSMetMod_qmax](#)

Examples

```
d <- 3
n <- 50;nT <- 50
library(lhs)
X <- maximinLHS(n, d);XT <- maximinLHS(nT, d)
c <- c(0.2,0.6,0.8)
F <- 1;for (a in 1:d) F <- F*(abs(4*X[,a]-2)+c[a])/(1+c[a])
FT <- 1;for (a in 1:d) FT <- FT*(abs(4*XT[,a]-2)+c[a])/(1+c[a])
sigma <- 0.2
epsilon <- rnorm(n,0,1);Y <- F + sigma*epsilon
epsilonT <- rnorm(nT,0,1);YT <- FT + sigma*epsilonT
Dmax <- 3
kernel <- "matern"
frc <- c(10)
gamma=c(.5,.01,.001)
res <- RKHSMetMod(Y,X,kernel,Dmax,gamma,frc,FALSE)
mu <- vector()
l <- length(gamma)
for(i in 1:length(frc)){mu[i]=res[[i-1]*l+1]}$mu}
error <- PredErr(X,XT, YT,mu,gamma, res, kernel,Dmax)
SI.minErr <- SI_emp(res, error)
SI.minErr
SI <- SI_emp(res, NULL)
SI
```

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