# <span id="page-0-0"></span>Package: KRLS (via r-universe)

October 18, 2024

Type Package

Title Kernel-Based Regularized Least Squares

Version 1.0-0

Date 2017-07-08

Author Jens Hainmueller (Stanford) Chad Hazlett (UCLA)

Maintainer Jens Hainmueller <jhain@stanford.edu>

Description Package implements Kernel-based Regularized Least Squares (KRLS), a machine learning method to fit multidimensional functions  $y=f(x)$  for regression and classification problems without relying on linearity or additivity assumptions. KRLS finds the best fitting function by minimizing the squared loss of a Tikhonov regularization problem, using Gaussian kernels as radial basis functions. For further details see Hainmueller and Hazlett (2014).

License GPL  $(>= 2)$ 

Suggests lattice

URL <https://www.r-project.org>, <https://www.stanford.edu/~jhain/>

NeedsCompilation no

Date/Publication 2017-07-10 13:55:59 UTC

Repository https://jankee2022.r-universe.dev

RemoteUrl https://github.com/cran/KRLS

RemoteRef HEAD

RemoteSha 9ee4980f0f951956294c84b7f49fe4374e5a432b

# **Contents**



#### <span id="page-1-0"></span>2 fdskrls



fdskrls *Compute first differences with KRLS*

# Description

Internal function that is called by [krls](#page-3-1) to computes first differences for binary predictors in the X matrix. It would normally not be called by the user directly.

# Usage

fdskrls(object,...)

# Arguments



# Value

A object of class krls where the derivatives, average derivatives, and the varinaces of the average derivatives are replaced with the first differences for binary predictors. The binaryindicator is also updated and set to TRUE for binary predictors.

# Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

### See Also

[krls](#page-3-1)

<span id="page-2-1"></span><span id="page-2-0"></span>

# Description

Given a  $N$  by  $D$  numeric data matrix, this function computes the  $N$  by  $N$  distance matrix with the pairwise distances between the rows of the data matrix as measured by a Gaussian Kernel.

#### Usage

```
gausskernel(X = NULL, sigma = NULL)
```
#### Arguments



#### Details

Given two D dimensional vectors  $x_i$  and  $x_j$ . The Gaussian kernel is defined as

$$
k(x_i, x_j) = exp(\frac{-||x_i - x_j||^2}{\sigma^2})
$$

where  $||x_i - x_j||$  is the Euclidean distance given by

$$
||x_i - x_j|| = ((x_i 1 - x_j 1)^2 + (x_i 2 - x_j 2)^2 + \dots + (x_i D - x_j D)^2)
$$

and  $\sigma^2$  is the bandwidth of the kernel.

Note that the Gaussian kernel is a measure of similarity between  $x_i$  and  $x_j$ . It evalues to 1 if the  $x_i$ and  $x_j$  are identical, and approaches 0 as  $x_i$  and  $x_j$  move further apart.

The function relies on the [dist](#page-0-0) function in the stats package for an initial estimate of the euclidean distance.

#### Value

An  $N$  by  $N$  numeric distance matrix that contains the pairwise distances between the rows in  $X$ .

# Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

#### See Also

[dist](#page-0-0) function in the stats package.

## <span id="page-3-0"></span>Examples

```
X \leftarrow matrix(rnorm(6),ncol=2)gausskernel(X=X,sigma=1)
```
<span id="page-3-1"></span>krls *Kernel-based Regularized Least Squares (KRLS)*

#### Description

Function implements Kernel-Based Regularized Least Squares (KRLS), a machine learning method described in Hainmueller and Hazlett (2014) that allows users to solve regression and classification problems without manual specification search and strong functional form assumptions. KRLS finds the best fitting function by minimizing a Tikhonov regularization problem with a squared loss, using Gaussian Kernels as radial basis functions. KRLS reduces misspecification bias since it learns the functional form from the data. Yet, it nevertheless allows for interpretability and inference in ways similar to ordinary regression models. In particular, KRLS provides closed-form estimates for the predicted values, variances, and the pointwise partial derivatives that characterize the marginal effects of each independent variable at each data point in the covariate space. The distribution of pointwise marginal effects can be used to examine effect heterogeneity and or interactions.

#### Usage

```
krls(X = NULL, y = NULL, whichkernel = "gaussian", lambda = NULL,sigma = NULL, derivative = TRUE, binary= TRUE, vcov=TRUE,
print.level = 1,L=NULL,U=NULL,tol=NULL,eigtrunc=NULL)
```


<span id="page-4-0"></span>

#### Details

krls implements the Kernel-based Regularized Least Squares (KRLS) estimator as described in Hainmueller and Hazlett (2014). Please consult this reference for any details.

Kernel-based Regularized Least Squares (KRLS) arises as a Tikhonov minimization problem with a squared loss. Assume we have data of the from  $y_i$ ,  $x_i$  where i indexes observations,  $y_i \in R$  is the outcome and  $x_i \in R^D$  is a D-dimensional vector of predictor values. Then KRLS searches over a space of functions  $H$  and chooses the best fitting function  $f$  according to the rule:

$$
argmin_{f \in H} \sum_{i}^{N} (y_i - f(x_i))^2 + \lambda ||f||_{H^2}
$$

where  $(y_i - f(x_i))^2$  is a loss function that computes how 'wrong' the function is at each observation i and  $||f||_{H^2}$  is the regularizer that measures the complexity of the function according to the  $L_2$ norm  $||f||^2 = \int f(x)^2 dx$ .  $\lambda$  is the scalar regularization parameter that governs the tradeoff between model fit and complexity. By default,  $\lambda$  is chosen by minimizing the sum of the squared leave-oneout errors, but it can also be specified by the user in the lambda argument to implement other approaches.

Under fairly general conditions, the function that minimizes the regularized loss within the hypothesis space established by the choice of a (positive semidefinite) kernel function  $k(x_i, x_j)$  is of the form

$$
f(x_j) = \sum_{i}^{N} c_i k(x_i, x_j)
$$

where the kernel function  $k(x_i, x_j)$  measures the distance between two observations  $x_i$  and  $x_j$ and  $c_i$  is the choice coefficient for each observation i. Let K be the N by N kernel matrix with all pairwise distances  $K_{i,j} = k(x_i, x_j)$  and c be the N by 1 vector of choice coefficients for all observations then in matrix notation the space is  $y = Kc$ .

Accordingly, the krls function solves the following minimization problem

$$
argmin_{f \in H} \sum_{i}^{n} (y - Kc)'(y - Kc) + \lambda c' Kc
$$

which is convex in c and solved by  $c = (K + \lambda I)^{-1}y$  where I is the identity matrix. Note that this linear solution provides a flexible fitted response surface that typically reduces misspecification bias because it can learn a wide range of nonlinear and or nonadditive functions of the predictors.

If vcov=TRUE is specified, krls also computes the variance-covariance matrix for the choice coefficients c and fitted values  $y = Kc$  based on a variance estimator developed in Hainmueller and Hazlett (2014). Note that both matrices are  $N$  by  $N$  and therefore this results in increased memory and computing time.

By default, krls uses the Gaussian Kernel (whichkernel = "gaussian") given by

$$
k(x_i, x_j) = exp(\frac{-||x_i - x_j||^2}{\sigma^2})
$$

where  $||x_i - x_j||$  is the Euclidean distance. The kernel bandwidth  $\sigma^2$  is set to D, the number of dimensions, by default, but the user can also specify other values using the sigma argument to implement other approaches.

If derivative=TRUE is specified, krls also computes the pointwise partial derivatives of the fitted function wrt to each predictor using the estimators developed in Hainmueller and Hazlett (2014). These can be used to examine the marginal effects of each predictor and how the marginal effects vary across the covariate space. Average derivatives are also computed with variances. Note that the derivative=TRUE option results in increased computing time and is only supported for the Gaussian kernel, i.e. when whichkernel = "gaussian". Also derivative=TRUE requires that vcov=TRUE.

If binary=TRUE is also specified, the function will identify binary predictors and return first differences for these predictors instead of partial derivatives. First differences are computed going from the minimum to the maximum value of each binary predictor. Note that first differences are more appropriate to summarize the effects for binary predictors (see Hainmueller and Hazlett (2014) for details).

A few other kernels are also implemented, but derivatives are currently not supported for these: "linear":  $k(x_i, x_j) = x'_i x_j$ , "poly1", "poly2", "poly3", "poly4" are polynomial kernels based on  $k(x_i, x_j) = (x'_i x_j + 1)^p$  where p is the order.

# Value

A list object of class krls with the following elements:



# Note

The function requires the storage of a  $N$  by  $N$  kernel matrix and can therefore exceed the memory limits for very large datasets.

Setting derivative=FALSE and vcov=FALSE is useful to reduce computing time if pointwise partial derivatives and or variance covariance matrices are not needed.

# Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

#### <span id="page-7-0"></span>References

Jeremy Ferwerda, Jens Hainmueller, Chad J. Hazlett (2017). Kernel-Based Regularized Least Squares in R (KRLS) and Stata (krls). Journal of Statistical Software, 79(3), 1-26. doi:10.18637/jss.v079.i03

Hainmueller, J. and Hazlett, C. (2014). Kernel Regularized Least Squares: Reducing Misspecification Bias with a Flexible and Interpretable Machine Learning Approach. Political Analysis, 22(2)

Rifkin, R. 2002. Everything Old is New Again: A fresh look at historical approaches in machine learning. Thesis, MIT. September, 2002.

Evgeniou, T., Pontil, M., and Poggio, T. (2000). Regularization networks and support vector machines. Advances In Computational Mathematics, 13(1):1-50.

Schoelkopf, B., Herbrich, R. and Smola, A.J. (2001) A generalized representer theorem. In 14th Annual Conference on Computational Learning Theory, pages 416-426.

Kimeldorf, G.S. Wahba, G. 1971. Some results on Tchebycheffian spline functions. Journal of Mathematical Analysis and Applications, 33:82-95.

#### See Also

[predict.krls](#page-12-1) for fitted values and predictions. [summary.krls](#page-15-1) for summary of the fit. [plot.krls](#page-11-1) for plots of the fit.

#### Examples

```
# Linear example
# set up data
N < -200x1 \leq -\text{rnorm}(N)x2 <- rbinom(N,size=1,prob=.2)
y \le -x1 + .5*x2 + rnorm(N, \emptyset, .15)X \leftarrow \text{cbind}(x1, x2)# fit model
krlsout <- krls(X=X,y=y)
# summarize marginal effects and contribution of each variable
summary(krlsout)
# plot marginal effects and conditional expectation plots
plot(krlsout)
# non-linear example
# set up data
N < -200x1 \leftarrow \text{rnorm}(N)x2 <- rbinom(N,size=1,prob=.2)
y \le -x1^3 + .5*x^2 + \text{rnorm}(N, \emptyset, .15)X \leftarrow \text{cbind}(x1, x2)# fit model
krlsout <- krls(X=X,y=y)
# summarize marginal effects and contribution of each variable
summary(krlsout)
```
## <span id="page-8-0"></span>lambdasearch 9

```
# plot marginal effects and conditional expectation plots
plot(krlsout)
## 2D example:
# predictor data
X \leftarrow matrix(seq(-3, 3, .1))# true function
Ytrue \leq -\sin(X)# add noise
      \le sin(X) + rnorm(length(X), sd=.3)
# approximate function using KRLS
out <- krls(y=Y,X=X)
# get fitted values and ses
fit <- predict(out,newdata=X,se.fit=TRUE)
# results
par(mfrow=c(2,1))
plot(y=Ytrue,x=X,type="l",col="red",ylim=c(-1.2,1.2),lwd=2,main="f(x)")
points(y=fit$fit,X,col="blue",pch=19)
arrows(y1=fit$fit+1.96*fit$se.fit,
       y0=fit$fit-1.96*fit$se.fit,
       x1=X,x0=X,col="blue",length=0)
legend("bottomright",legend=c("true f(x)=sin(x)","KRLS fitted f(x)"),
       lty=c(1,NA),pch=c(NA,19),lwd=c(2,NA),col=c("red","blue"),cex=.8)
plot(y=cos(X),x=X,type="l",col="red",ylim=c(-1.2,1.2),lwd=2,main="df(x)/dx")
points(y=out$derivatives,X,col="blue",pch=19)
legend("bottomright",legend=c("true df(x)/dx=cos(x)","KRLS fitted df(x)/dx"),
       lty=c(1,NA),pch=c(NA,19),lwd=c(2,NA),col=c("red","blue"),,cex=.8)
## 3D example
# plot true function
par(mfrow=c(1,2))
f <-function(x1,x2){ sin(x1)*cos(x2)}
x1 \leftarrow x2 \leftarrow seq(0, 2*pi, .2)z \quad \text{--outer}(x1, x2, f)persp(x1, x2, z,theta=30,main="true f(x1,x2)=sin(x1)cos(x2)")
# approximate function with KRLS
# data and outcomes
X <- cbind(sample(x1,200,replace=TRUE),sample(x2,200,replace=TRUE))
y <- f(X[,1],X[,2])+ runif(nrow(X))
# fit surface
krlsout <- krls(X=X,y=y)
# plot fitted surface
ff <- function(x1i,x2i,krlsout){predict(object=krlsout,newdata=cbind(x1i,x2i))$fit}
z <- outer(x1,x2,ff,krlsout=krlsout)
persp(x1, x2, z,theta=30,main="KRLS fitted f(x1,x2)")
```
<span id="page-8-1"></span>lambdasearch *Leave-one-out optimization to find* λ

#### <span id="page-9-0"></span>Description

Function conducts leave-one-out optimization to find  $\lambda$  using a golden search search with caching. This function is called internally by [krls](#page-3-1). It would normally not be called by the user directly.

#### Usage

```
lambdasearch(L=NULL,
           U=NULL,
           y=NULL,
           Eigenobject=NULL,
           tol=NULL,
           noisy=FALSE,
           eigtrunc=NULL)
```
## Arguments



#### Details

By default, upper bound is found as follows: Set j to n, decrease by one until the following is longer true: sum(EigenValues / (EigenValues + j)) < 1.

By default, upper bound is found as follows: Get the position, q, of the eigenvalue that is closest to max(Eigenvalue)/1000. Set j to 0, increase in steps of 0.05 until the below is longer true: sum(EigenValues / (EigenValues + j)) > q.

# Value

A scalar that contains the  $\lambda$  that minimizes the sum of squared leave-one-out errors.

#### Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

#### <span id="page-10-0"></span>looloss and the set of t

# See Also

[krls](#page-3-1)

looloss *Loss Function for Leave One Out Error*

# Description

Internal function that computes Leave-On-Out (LOO) Error for KRLS given a fixed value for lambda (the parameter that governs the tradeoff between model fit and complexity in KRLS). This function is called internally by krls to find value of lambda that minimizes the LOO error. It would normally not be called by the user directly.

# Usage

looloss(y = NULL, Eigenobject = NULL, lambda = NULL,eigtrunc=NULL)

# Arguments



#### Value

Scalar value for LOO error.

#### Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

#### See Also

[krls](#page-3-1)

<span id="page-11-1"></span><span id="page-11-0"></span>

# Description

Produces two types of plots. The first type of plot shows histograms for the pointwise partial derivatives to examine the heterogeneity in the marginal effects of each predictor (which==1). The second type of plot shows estimates of the conditional expectation functions of  $E[Y|X]$  for each predictor (which==2). For each plot, the predictor of interest varies from its 1st to its 3rd quartile values, while the other predictors are kept at the means (or other values specified in setx). For binary varibales the  $E[Y|X]$  are predicted at the max and the min value of the predictor (instead of the range from the 1st to the 3rd quantile).

#### Usage

```
## S3 method for class 'krls'
plot(x,which=c(1:2),
main="distributions of pointwise marginal effects",
setx="mean",ask = prod(par("mfcol")) < nplots,nvalues=50,probs=c(.25,.75),...)
```
# Arguments



#### Details

Notice that the historgrams for the partial derivatives can only be plotted if the KRLS object was computed with krls(,derivatives=TRUE).

# <span id="page-12-0"></span>predict.krls 13

# Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

#### See Also

[krls](#page-3-1)

# Examples

```
# non-linear example
# set up data
N < -200x1 \leftarrow \text{norm}(N)x2 <- rbinom(N,size=1,prob=.2)
y \le -x1^3 + .5*x2 + rnorm(N, \emptyset, .15)X \leftarrow \text{cbind}(x1, x2)# fit model
krlsout <- krls(X=X,y=y)
# summarize marginal effects and contribution of each variable
summary(krlsout)
# plot marginal effects and conditional expectation plots
plot(krlsout)
```
<span id="page-12-1"></span>

# Description

Predicted values and standard errors based on krls model object.

#### Usage

```
## S3 method for class 'krls'
predict(object, new data, se.fit = FALSE, ...)
```


#### Details

Function produces predicted values, obtained by evaluating the fitted krls function with the newdata (ie. the test points). The prediction at a new test point  $x_i$  is based on

$$
f(x_i) = \sum_j \frac{1}{i} n c_j K_{x_j}(x_i)
$$

where K is the kernel matrix and thus  $K_{x_j}$  is a vector whose j-th entry is  $K(x_j, x_i)$  (e.g. the distance between the test point  $x_i$  and the training point  $x_j$ ). The training points are passed to the function with the krls fit in object.

When data are missing in newdata during prediction, the value of each  $k(x_i, x_j)$  is computed by using an adjusted Euclidean distance in the kernel definition. Assume  $x$  is  $D$ -dimensional but a given pair of observations  $x_i$  and  $x_j$  have only  $D' < D$  non-missing dimensions in common. The adjusted Euclidean distance computes the sum of squared differences over the  $D'$  non-missing dimensions, rescales this sum by  $D/D'$ , and takes the square root. The result corresponds to an assumption that conditional on the observed data, the missing values would not have contributed new information predictive of the outcome.

#### Value



#### Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

#### See Also

[krls](#page-3-1)

#### Examples

```
# make up data
X \leftarrow \text{seq}(-3, 3, .1)Y \leftarrow \sin(X) + \text{norm}(\text{length}(X), .1)# fit krls
krlsout <- krls(y=Y,X=X)
# get in-sample prediction
```
predin <- predict(krlsout,newdata=X,se.fit=TRUE)

#### <span id="page-14-0"></span>solveforc and the solvetic state of the solvet

```
# get out-of-sample prediction
X2 \leftarrow runif(5)predout <- predict(krlsout,newdata=X2,se.fit=TRUE)
# plot true function and predictions
plot(y=sin(X),x=X,type="1",col="red",ylim=c(-1.8,1.8),lwd=2,ylab="f(X)")points(y=predin$fit,x=X,col="blue",pch=19)
arrows(y1=predin$fit+2*predin$se.fit,
       y0=predin$fit-2*predin$se.fit,
       x1=X,x0=X,col="blue",length=0)
points(y=predout$fit,x=X2,col="green",pch=17)
arrows(y1=predout$fit+2*predout $se.fit,
       y0=predout$fit-2*predout $se.fit,
       x1=X2,x0=X2,col="green",length=0)
legend("bottomright",
       legend=c("true f(x)=sin(X)",
                "KRLS fitted in-sample",
                "KRLS fitted out-of-sample"),
       lty=c(1,NA,NA),pch=c(NA,19,17),
       lwd=c(2,NA,NA),
       col=c("red","blue","green"),
       cex=.8)
```
solveforc *Solve for Choice Coefficients in KRLS*

# Description

Internal function that computes choice coefficients for KRLS given a fixed value for lambda (the parameter that governs the tradeoff between model fit and complexity in KRLS). This function is called internally by [krls](#page-3-1). It would normally not be called by the user directly.

#### Usage

 $solveforce(y = NULL, Eigenobject = NULL,$ lambda = NULL,eigtrunc=NULL)



# Details

Function relies on fast eigenvalue decomposition method described in method Rifkin and Lippert (2007).

#### Value



## Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

## References

Rifkin, Ryan M. and Lippert, Ross A. (2007). Notes on Regularized Least Squares. MIT-CSAIL-TR-2007-025. CBCL-268

# See Also

[krls](#page-3-1)

<span id="page-15-1"></span>

# Description

Summarizes average partial derivatives (i.e. marginal effects) and the distribution of the partial derivatives for each predictor. For binary predictors, the marginal effects are the first differences if krls(,derivatives=TRUE,binary=TRUE) was specified.

# Usage

```
## S3 method for class 'krls'
summary(object, probs=c(.25,.5,.75),...)
```


<span id="page-15-0"></span>

# <span id="page-16-0"></span>summary.krls 17

# Details

Notice that the partial derivatives can only be summarized if the krls object was computed with krls(,derivatives=TRUE).

#### Value



# Author(s)

Jens Hainmueller (Stanford) and Chad Hazlett (MIT)

# See Also

[krls](#page-3-1)

### Examples

```
# non-linear example
# set up data
N < -200x1 \leftarrow \text{norm}(N)x2 <- rbinom(N,size=1,prob=.2)
y \le -x1^3 + .5*x2 + rnorm(N, \emptyset, .15)X \leftarrow \text{cbind}(x1, x2)# fit model
krlsout <- krls(X=X,y=y)
```

```
# summarize marginal effects and contribution of each variable
summary(krlsout)
# plot marginal effects and conditional expectation plots
plot(krlsout)
```
# <span id="page-17-0"></span>Index

∗ multivariate, smooth, kernels, machine learning, regression, classification krls, [4](#page-3-0) dist, *[3](#page-2-0)* eigen, *[15](#page-14-0)* fdskrls, [2](#page-1-0) gausskernel, [3,](#page-2-0) *[4](#page-3-0)* krls, *[2](#page-1-0)*, [4,](#page-3-0) *[10](#page-9-0)[–17](#page-16-0)* lambdasearch, *[5](#page-4-0)*, [9](#page-8-0) looloss, [11](#page-10-0) par, *[12](#page-11-0)* plot.krls, *[8](#page-7-0)*, [12](#page-11-0) predict.krls, *[8](#page-7-0)*, [13](#page-12-0) quantile, *[16](#page-15-0)*

solveforc, [15](#page-14-0) summary.krls, *[8](#page-7-0)*, [16](#page-15-0)