# Package 'kernlab'

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as.kernelMatrix

Assing kernelMatrix class to matrix objects

### **Description**

as.kernelMatrix in package **kernlab** can be used to coerce the kernelMatrix class to matrix objects representing a kernel matrix. These matrices can then be used with the kernelMatrix interfaces which most of the functions in **kernlab** support.

# Usage

```
## S4 method for signature 'matrix'
as.kernelMatrix(x, center = FALSE)
```

### **Arguments**

x matrix to be assigned the kernelMatrix class
center center the kernel matrix in feature space (default: FALSE)

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# See Also

```
kernelMatrix, dots
```

```
## Create toy data
x <- rbind(matrix(rnorm(10),,2),matrix(rnorm(10,mean=3),,2))
y <- matrix(c(rep(1,5),rep(-1,5)))

### Use as.kernelMatrix to label the cov. matrix as a kernel matrix
### which is eq. to using a linear kernel

K <- as.kernelMatrix(crossprod(t(x)))

K

svp2 <- ksvm(K, y, type="C-svc")

svp2</pre>
```

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couple

Probabilities Coupling function

### **Description**

couple is used to link class-probability estimates produced by pairwise coupling in multi-class classification problems.

### Usage

```
couple(probin, coupler = "minpair")
```

# **Arguments**

probin The pairwise coupled class-probability estimates

coupler The type of coupler to use. Currently minpar and pkpd and vote are supported

(see reference for more details). If vote is selected the returned value is a prim-

itive estimate passed on given votes.

#### **Details**

As binary classification problems are much easier to solve many techniques exist to decompose multi-class classification problems into many binary classification problems (voting, error codes, etc.). Pairwise coupling (one against one) constructs a rule for discriminating between every pair of classes and then selecting the class with the most winning two-class decisions. By using Platt's probabilities output for SVM one can get a class probability for each of the k(k-1)/2 models created in the pairwise classification. The couple method implements various techniques to combine these probabilities.

#### Value

A matrix with the resulting probability estimates.

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### References

```
Ting-Fan Wu, Chih-Jen Lin, ruby C. Weng
Probability Estimates for Multi-class Classification by Pairwise Coupling
Neural Information Processing Symposium 2003
```

https://papers.neurips.cc/paper/2454-probability-estimates-for-multi-class-classification-by-pairw pdf

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### See Also

```
predict.ksvm, ksvm
```

### **Examples**

```
## create artificial pairwise probabilities
pairs <- matrix(c(0.82,0.12,0.76,0.1,0.9,0.05),2)
couple(pairs)
couple(pairs, coupler="pkpd")
couple(pairs, coupler = "vote")</pre>
```

csi

Cholesky decomposition with Side Information

### Description

The csi function in **kernlab** is an implementation of an incomplete Cholesky decomposition algorithm which exploits side information (e.g., classification labels, regression responses) to compute a low rank decomposition of a kernel matrix from the data.

# Usage

```
## S4 method for signature 'matrix'
csi(x, y, kernel="rbfdot", kpar=list(sigma=0.1), rank,
centering = TRUE, kappa = 0.99 ,delta = 40 ,tol = 1e-5)
```

#### **Arguments**

Χ

The data matrix indexed by row

У

the classification labels or regression responses. In classification y is a  $m \times n$  matrix where m the number of data and n the number of classes y and  $y_i$  is 1 if the corresponding x belongs to class i.

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes the inner product in feature space between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function

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- anovadot ANOVA RBF kernel function
- splinedot Spline kernel
- stringdot String kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

rank maximal rank of the computed kernel matrix centering if TRUE centering is performed (default: TRUE)

kappa trade-off between approximation of K and prediction of Y (default: 0.99) number of columns of cholesky performed in advance (default: 40)

tol minimum gain at each iteration (default: 1e-4)

#### **Details**

An incomplete cholesky decomposition calculates Z where K = ZZ' K being the kernel matrix. Since the rank of a kernel matrix is usually low, Z tends to be smaller then the complete kernel matrix. The decomposed matrix can be used to create memory efficient kernel-based algorithms without the need to compute and store a complete kernel matrix in memory.

csi uses the class labels, or regression responses to compute a more appropriate approximation for the problem at hand considering the additional information from the response variable.

#### Value

An S4 object of class "csi" which is an extension of the class "matrix". The object is the decomposed kernel matrix along with the slots :

pivots Indices on which pivots where done

diagresidues Residuals left on the diagonal maxresiduals Residuals picked for pivoting

predgain predicted gain before adding each column actual gain after adding each column

Q QR decomposition of the kernel matrix

R QR decomposition of the kernel matrix

slots can be accessed either by object@slot or by accessor functions with the same name (e.g., pivots(object))

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### Author(s)

```
Alexandros Karatzoglou (based on Matlab code by Francis Bach) <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# References

```
Francis R. Bach, Michael I. Jordan

Predictive low-rank decomposition for kernel methods.

Proceedings of the Twenty-second International Conference on Machine Learning (ICML) 2005

http://www.di.ens.fr/~fbach/bach_jordan_csi.pdf
```

#### See Also

```
inchol, chol, csi-class
```

# **Examples**

```
data(iris)
## create multidimensional y matrix
yind <- t(matrix(1:3,3,150))
ymat <- matrix(0, 150, 3)
ymat[yind==as.integer(iris[,5])] <- 1

datamatrix <- as.matrix(iris[,-5])
# initialize kernel function
rbf <- rbfdot(sigma=0.1)
rbf
Z <- csi(datamatrix,ymat, kernel=rbf, rank = 30)
dim(Z)
pivots(Z)
# calculate kernel matrix
K <- crossprod(t(Z))
# difference between approximated and real kernel matrix
(K - kernelMatrix(kernel=rbf, datamatrix))[6,]</pre>
```

csi-class

Class "csi"

# **Description**

The reduced Cholesky decomposition object

# **Objects from the Class**

Objects can be created by calls of the form new("csi", ...). or by calling the csi function.

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#### Slots

```
.Data: Object of class "matrix" contains the decomposed matrix

pivots: Object of class "vector" contains the pivots performed

diagresidues: Object of class "vector" contains the diagonial residues

maxresiduals: Object of class "vector" contains the maximum residues

predgain Object of class "vector" contains the predicted gain before adding each column

truegain Object of class "vector" contains the actual gain after adding each column

Q Object of class "matrix" contains Q from the QR decomposition of the kernel matrix

R Object of class "matrix" contains R from the QR decomposition of the kernel matrix
```

#### **Extends**

```
Class "matrix", directly.
```

#### Methods

```
diagresidues signature(object = "csi"): returns the diagonial residues
maxresiduals signature(object = "csi"): returns the maximum residues
pivots signature(object = "csi"): returns the pivots performed
predgain signature(object = "csi"): returns the predicted gain before adding each column
truegain signature(object = "csi"): returns the actual gain after adding each column
Q signature(object = "csi"): returns Q from the QR decomposition of the kernel matrix
R signature(object = "csi"): returns R from the QR decomposition of the kernel matrix
```

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# See Also

```
csi, inchol-class
```

```
data(iris)
## create multidimensional y matrix
yind <- t(matrix(1:3,3,150))
ymat <- matrix(0, 150, 3)
ymat[yind==as.integer(iris[,5])] <- 1

datamatrix <- as.matrix(iris[,-5])
# initialize kernel function
rbf <- rbfdot(sigma=0.1)
rbf</pre>
```

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```
Z <- csi(datamatrix,ymat, kernel=rbf, rank = 30)</pre>
pivots(Z)
# calculate kernel matrix
K <- crossprod(t(Z))</pre>
# difference between approximated and real kernel matrix
(K - kernelMatrix(kernel=rbf, datamatrix))[6,]
```

dots

Kernel Functions

# **Description**

```
The kernel generating functions provided in kernlab.
The Gaussian RBF kernel k(x, x') = \exp(-\sigma ||x - x'||^2)
The Polynomial kernel k(x, x') = (scale < x, x' > +offset)^{degree}
The Linear kernel k(x, x') = \langle x, x' \rangle
The Hyperbolic tangent kernel k(x, x') = \tanh(scale < x, x' > + offset)
The Laplacian kernel k(x, x') = \exp(-\sigma ||x - x'||)
The Bessel kernel k(x, x') = (-Bessel^n_{(\nu+1)}\sigma \|x - x'\|^2)
The ANOVA RBF kernel k(x,x') = \sum_{1 \le i_1 \dots < i_D \le N} \prod_{d=1}^D k(x_{id},x'_{id}) where k(x,x) is a Gaussian
RBF kernel.
```

The Spline kernel  $\prod_{d=1}^D 1 + x_i x_j + x_i x_j min(x_i, x_j) - \frac{x_i + x_j}{2} min(x_i, x_j)^2 + \frac{min(x_i, x_j)^3}{3} \setminus \text{The Spline kernel}$ String kernels (see stringdot.

# Usage

```
rbfdot(sigma = 1)
polydot(degree = 1, scale = 1, offset = 1)
tanhdot(scale = 1, offset = 1)
vanilladot()
laplacedot(sigma = 1)
besseldot(sigma = 1, order = 1, degree = 1)
anovadot(sigma = 1, degree = 1)
splinedot()
```

#### **Arguments**

sigma

The inverse kernel width used by the Gaussian the Laplacian, the Bessel and the ANOVA kernel

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degree	The degree of the polynomial, bessel or ANOVA kernel function. This has to be an positive integer.
scale	The scaling parameter of the polynomial and tangent kernel is a convenient way of normalizing patterns without the need to modify the data itself
offset	The offset used in a polynomial or hyperbolic tangent kernel
order	The order of the Bessel function to be used as a kernel

#### **Details**

The kernel generating functions are used to initialize a kernel function which calculates the dot (inner) product between two feature vectors in a Hilbert Space. These functions can be passed as a kernel argument on almost all functions in **kernlab**(e.g., ksvm, kpca etc).

Although using one of the existing kernel functions as a kernel argument in various functions in **kernlab** has the advantage that optimized code is used to calculate various kernel expressions, any other function implementing a dot product of class kernel can also be used as a kernel argument. This allows the user to use, test and develop special kernels for a given data set or algorithm. For details on the string kernels see stringdot.

#### Value

Return an S4 object of class kernel which extents the function class. The resulting function implements the given kernel calculating the inner (dot) product between two vectors.

kpar a list containing the kernel parameters (hyperparameters) used.

The kernel parameters can be accessed by the kpar function.

### Note

If the offset in the Polynomial kernel is set to \$0\$, we obtain homogeneous polynomial kernels, for positive values, we have inhomogeneous kernels. Note that for negative values the kernel does not satisfy Mercer's condition and thus the optimizers may fail.

In the Hyperbolic tangent kernel if the offset is negative the likelihood of obtaining a kernel matrix that is not positive definite is much higher (since then even some diagonal elements may be negative), hence if this kernel has to be used, the offset should always be positive. Note, however, that this is no guarantee that the kernel will be positive.

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
stringdot, kernelMatrix, kernelMult, kernelPol
```

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### **Examples**

```
rbfkernel <- rbfdot(sigma = 0.1)
rbfkernel
kpar(rbfkernel)
## create two vectors
x <- rnorm(10)
y <- rnorm(10)
## calculate dot product
rbfkernel(x,y)</pre>
```

gausspr

Gaussian processes for regression and classification

# Description

gausspr is an implementation of Gaussian processes for classification and regression.

# Usage

# Arguments

х	a symbolic description of the model to be fit or a matrix or vector when a formula interface is not used. When not using a formula x is a matrix or vector containing the variables in the model
data	an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'gausspr' is called from.
у	a response vector with one label for each row/component of x. Can be either a factor (for classification tasks) or a numeric vector (for regression).

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type

Type of problem. Either "classification" or "regression". Depending on whether y is a factor or not, the default setting for type is classification or regression, respectively, but can be overwritten by setting an explicit value.

scaled

A logical vector indicating the variables to be scaled. If scaled is of length 1, the value is recycled as many times as needed and all non-binary variables are scaled. Per default, data are scaled internally (both x and y variables) to zero mean and unit variance. The center and scale values are returned and used for later predictions.

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are:

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

var

the initial noise variance, (only for regression) (default: 0.001)

variance.model

build model for variance or standard deviation estimation (only for regression) (default : FALSE)

tol

tolerance of termination criterion (default: 0.001)

fit

indicates whether the fitted values should be computed and included in the model or not (default: 'TRUE')

cross

if a integer value k>0 is specified, a k-fold cross validation on the training data is performed to assess the quality of the model: the Mean Squared Error for regression

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subset An index vector specifying the cases to be used in the training sample. (NOTE:

If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

... additional parameters

#### **Details**

A Gaussian process is specified by a mean and a covariance function. The mean is a function of x (which is often the zero function), and the covariance is a function C(x,x') which expresses the expected covariance between the value of the function y at the points x and x'. The actual function y(x) in any data modeling problem is assumed to be a single sample from this Gaussian distribution. Laplace approximation is used for the parameter estimation in gaussian processes for classification.

The predict function can return class probabilities for classification problems by setting the type parameter to "probabilities". For the regression setting the type parameter to "variance" or "sdeviation" returns the estimated variance or standard deviation at each predicted point.

### Value

An S4 object of class "gausspr" containing the fitted model along with information. Accessor functions can be used to access the slots of the object which include:

alpha The resulting model parameters error Training error (if fit == TRUE)

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### References

C. K. I. Williams and D. Barber

Bayesian classification with Gaussian processes.

IEEE Transactions on Pattern Analysis and Machine Intelligence, 20(12):1342-1351, 1998

https://homepages.inf.ed.ac.uk/ckiw/postscript/pami\_final.ps.gz

#### See Also

```
predict.gausspr, rvm, ksvm, gausspr-class, lssvm
```

```
# train model
data(iris)
test <- gausspr(Species~.,data=iris,var=2)</pre>
```

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```
test
alpha(test)
# predict on the training set
predict(test,iris[,-5])
# class probabilities
predict(test, iris[,-5], type="probabilities")
# create regression data
x < - seq(-20, 20, 0.1)
y < -\sin(x)/x + rnorm(401, sd=0.03)
# regression with gaussian processes
foo <- gausspr(x, y)</pre>
foo
# predict and plot
ytest <- predict(foo, x)</pre>
plot(x, y, type = "1")
lines(x, ytest, col="red")
#predict and variance
x = c(-4, -3, -2, -1, 0, 0.5, 1, 2)
y = c(-2, 0, -0.5, 1, 2, 1, 0, -1)
plot(x,y)
foo2 <- gausspr(x, y, variance.model = TRUE)</pre>
xtest <- seq(-4,2,0.2)
lines(xtest, predict(foo2, xtest))
lines(xtest,
      predict(foo2, xtest)+2*predict(foo2,xtest, type="sdeviation"),
      col="red")
lines(xtest,
      predict(foo2, xtest)-2*predict(foo2,xtest, type="sdeviation"),
      col="red")
```

gausspr-class

Class "gausspr"

# **Description**

The Gaussian Processes object class

# **Objects from the Class**

Objects can be created by calls of the form new("gausspr", ...). or by calling the gausspr function

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#### Slots

```
tol: Object of class "numeric" contains tolerance of termination criteria
kernelf: Object of class "kfunction" contains the kernel function used
kpar: Object of class "list" contains the kernel parameter used
kcall: Object of class "list" contains the used function call
type: Object of class "character" contains type of problem
terms: Object of class "ANY" contains the terms representation of the symbolic model used (when
     using a formula)
xmatrix: Object of class "input" containing the data matrix used
ymatrix: Object of class "output" containing the response matrix
fitted: Object of class "output" containing the fitted values
lev: Object of class "vector" containing the levels of the response (in case of classification)
nclass: Object of class "numeric" containing the number of classes (in case of classification)
alpha: Object of class "listI" containing the computes alpha values
alphaindex Object of class "list" containing the indexes for the alphas in various classes (in
     multi-class problems).
sol Object of class "matrix" containing the solution to the Gaussian Process formulation, it is
     used to compute the variance in regression problems.
scaling Object of class "ANY" containing the scaling coefficients of the data (when case scaled =
     TRUE is used).
nvar: Object of class "numeric" containing the computed variance
error: Object of class "numeric" containing the training error
cross: Object of class "numeric" containing the cross validation error
n.action: Object of class "ANY" containing the action performed in NA
```

### Methods

```
alpha signature(object = "gausspr"): returns the alpha vector
cross signature(object = "gausspr"): returns the cross validation error
error signature(object = "gausspr"): returns the training error
fitted signature(object = "vm"): returns the fitted values
kcall signature(object = "gausspr"): returns the call performed
kernelf signature(object = "gausspr"): returns the kernel function used
kpar signature(object = "gausspr"): returns the kernel parameter used
lev signature(object = "gausspr"): returns the response levels (in classification)
type signature(object = "gausspr"): returns the type of problem
xmatrix signature(object = "gausspr"): returns the data matrix used
ymatrix signature(object = "gausspr"): returns the response matrix used
scaling signature(object = "gausspr"): returns the scaling coefficients of the data (when scaled
    = TRUE is used)
```

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### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
gausspr, ksvm-class, vm-class
```

### **Examples**

```
# train model
data(iris)
test <- gausspr(Species~.,data=iris,var=2)
test
alpha(test)
error(test)
lev(test)</pre>
```

inchol

Incomplete Cholesky decomposition

### **Description**

inchol computes the incomplete Cholesky decomposition of the kernel matrix from a data matrix.

### Usage

# Arguments

--

The data matrix indexed by row

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes the inner product in feature space between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel

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> The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

the list of hyper-parameters (kernel parameters). This is a list which contains kpar

the parameters to be used with the kernel function. Valid parameters for existing

kernels are:

• sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".

• degree, scale, offset for the Polynomial kernel "polydot"

• scale, offset for the Hyperbolic tangent kernel function "tanhdot"

• sigma, order, degree for the Bessel kernel "besseldot".

• sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

tol algorithm stops when remaining pivots bring less accuracy then tol (default:

maxiter maximum number of iterations and columns in Zadd this many columns to matrix per iteration blocksize

print info on algorithm convergence verbose

#### **Details**

An incomplete cholesky decomposition calculates Z where K = ZZ' K being the kernel matrix. Since the rank of a kernel matrix is usually low, Z tends to be smaller then the complete kernel matrix. The decomposed matrix can be used to create memory efficient kernel-based algorithms without the need to compute and store a complete kernel matrix in memory.

#### Value

An S4 object of class "inchol" which is an extension of the class "matrix". The object is the decomposed kernel matrix along with the slots:

pivots Indices on which pivots where done diagresidues Residuals left on the diagonal maxresiduals Residuals picked for pivoting

slots can be accessed either by object@slot or by accessor functions with the same name (e.g., pivots(object))

### Author(s)

Alexandros Karatzoglou (based on Matlab code by S.V.N. (Vishy) Vishwanathan and Alex Smola) <alexandros.karatzoglou@ci.tuwien.ac.at>

#### References

Francis R. Bach, Michael I. Jordan Kernel Independent Component Analysis Journal of Machine Learning Research 3, 1-48

https://www.jmlr.org/papers/volume3/bach02a/bach02a.pdf

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### See Also

```
csi, inchol-class, chol
```

### **Examples**

```
data(iris)
datamatrix <- as.matrix(iris[,-5])
# initialize kernel function
rbf <- rbfdot(sigma=0.1)
rbf
Z <- inchol(datamatrix,kernel=rbf)
dim(Z)
pivots(Z)
# calculate kernel matrix
K <- crossprod(t(Z))
# difference between approximated and real kernel matrix
(K - kernelMatrix(kernel=rbf, datamatrix))[6,]</pre>
```

inchol-class

Class "inchol"

# Description

The reduced Cholesky decomposition object

# **Objects from the Class**

Objects can be created by calls of the form new("inchol", ...). or by calling the inchol function.

#### **Slots**

```
.Data: Object of class "matrix" contains the decomposed matrix pivots: Object of class "vector" contains the pivots performed diagresidues: Object of class "vector" contains the diagonial residues maxresiduals: Object of class "vector" contains the maximum residues
```

### **Extends**

```
Class "matrix", directly.
```

#### Methods

```
diagresidues signature(object = "inchol"): returns the diagonial residues
maxresiduals signature(object = "inchol"): returns the maximum residues
pivots signature(object = "inchol"): returns the pivots performed
```

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# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# See Also

```
inchol, csi-class, csi
```

# **Examples**

```
data(iris)
datamatrix <- as.matrix(iris[,-5])
# initialize kernel function
rbf <- rbfdot(sigma=0.1)
rbf
Z <- inchol(datamatrix,kernel=rbf)
dim(Z)
pivots(Z)
diagresidues(Z)
maxresiduals(Z)</pre>
```

income

Income Data

# Description

Customer Income Data from a marketing survey.

# Usage

```
data(income)
```

# **Format**

A data frame with 14 categorical variables (8993 observations).

Explanation of the variable names:

1	INCOME	annual income of household	
		(Personal income if single)	ordinal
2	SEX	sex	nominal
3	MARITAL.STATUS	marital status	nominal
4	AGE	age	ordinal
5	EDUCATION	educational grade	ordinal
6	OCCUPATION	type of work	nominal
7	AREA	how long the interviewed person has lived	
		in the San Francisco/Oakland/San Jose area	ordinal
8	DUAL.INCOMES	dual incomes (if married)	nominal

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9	HOUSEHOLD.SIZE	persons living in the household	ordinal
10	UNDER18	persons in household under 18	ordinal
11	HOUSEHOLDER	householder status	nominal
12	HOME.TYPE	type of home	nominal
13	ETHNIC.CLASS	ethnic classification	nominal
14	LANGUAGE	language most often spoken at home	nominal

#### **Details**

A total of N=9409 questionnaires containing 502 questions were filled out by shopping mall customers in the San Francisco Bay area. The dataset is an extract from this survey. It consists of 14 demographic attributes. The dataset is a mixture of nominal and ordinal variables with a lot of missing data. The goal is to predict the Anual Income of Household from the other 13 demographics attributes.

#### Source

Impact Resources, Inc., Columbus, OH (1987).

inlearn

Onlearn object initialization

### Description

Online Kernel Algorithm object onlearn initialization function.

### Usage

### **Arguments**

d

the dimensionality of the data to be learned

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function

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• anovadot ANOVA RBF kernel function

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. For valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

type

the type of problem to be learned by the online algorithm: classification,

 ${\it regression}, {\it novelty}$ 

buffersize

the size of the buffer to be used

#### **Details**

The inlearn is used to initialize a blank onlearn object.

### Value

The function returns an S4 object of class onlearn that can be used by the onlearn function.

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# See Also

```
onlearn, onlearn-class
```

ipop

```
sign(predict(on,x))
```

ipop

Quadratic Programming Solver

# Description

```
ipop solves the quadratic programming problem : \min(c'*x+1/2*x'*H*x) subject to: b<=A*x<=b+r l<=x<=u
```

# Usage

```
ipop(c, H, A, b, 1, u, r, sigf = 7, maxiter = 40, margin = 0.05, bound = 10, verb = 0)
```

# Arguments

С	Vector or one column matrix appearing in the quadratic function
Н	square matrix appearing in the quadratic function, or the decomposed form $Z$ of the $H$ matrix where $Z$ is a $nxm$ matrix with $n>m$ and $ZZ'=H$ .
A	Matrix defining the constrains under which we minimize the quadratic function
b	Vector or one column matrix defining the constrains
1	Lower bound vector or one column matrix
u	Upper bound vector or one column matrix
r	Vector or one column matrix defining constrains
sigf	Precision (default: 7 significant figures)
maxiter	Maximum number of iterations
margin	how close we get to the constrains
bound	Clipping bound for the variables
verb	Display convergence information during runtime

# **Details**

ipop uses an interior point method to solve the quadratic programming problem.

The H matrix can also be provided in the decomposed form Z where ZZ'=H in that case the Sherman Morrison Woodbury formula is used internally.

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### Value

An S4 object with the following slots

primal Vector containing the primal solution of the quadratic problem

dual The dual solution of the problem

how Character string describing the type of convergence

all slots can be accessed through accessor functions (see example)

### Author(s)

#### References

```
R. J. Vanderbei
```

```
LOQO: An interior point code for quadratic programming Optimization Methods and Software 11, 451-484, 1999 https://vanderbei.princeton.edu/ps/loqo5.pdf
```

#### See Also

```
solve.QP, inchol, csi
```

```
## solve the Support Vector Machine optimization problem
data(spam)
## sample a scaled part (500 points) of the spam data set
m < -500
set <- sample(1:dim(spam)[1],m)</pre>
x <- scale(as.matrix(spam[,-58]))[set,]</pre>
y <- as.integer(spam[set,58])</pre>
y[y==2] <- -1
##set C parameter and kernel
rbf <- rbfdot(sigma = 0.1)</pre>
## create H matrix etc.
H <- kernelPol(rbf,x,,y)</pre>
c <- matrix(rep(-1,m))</pre>
A \leftarrow t(y)
b <- 0
1 <- matrix(rep(0,m))</pre>
u <- matrix(rep(C,m))</pre>
r <- 0
sv \leftarrow ipop(c,H,A,b,l,u,r)
```

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```
sv
dual(sv)
```

ipop-class

Class "ipop"

# Description

The quadratic problem solver class

# **Objects from the Class**

Objects can be created by calls of the form new("ipop", ...). or by calling the ipop function.

### **Slots**

```
primal: Object of class "vector" the primal solution of the problem
dual: Object of class "numeric" the dual of the problem
how: Object of class "character" convergence information
```

### Methods

```
primal signature(object = "ipop"): Return the primal of the problem
dual signature(object = "ipop"): Return the dual of the problem
how signature(object = "ipop"): Return information on convergence
```

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# See Also

ipop

```
## solve the Support Vector Machine optimization problem
data(spam)

## sample a scaled part (300 points) of the spam data set
m <- 300
set <- sample(1:dim(spam)[1],m)
x <- scale(as.matrix(spam[,-58]))[set,]
y <- as.integer(spam[set,58])
y[y==2] <- -1</pre>
```

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```
##set C parameter and kernel
C <- 5
rbf <- rbfdot(sigma = 0.1)

## create H matrix etc.
H <- kernelPol(rbf,x,,y)
c <- matrix(rep(-1,m))
A <- t(y)
b <- 0
1 <- matrix(rep(0,m))
u <- matrix(rep(C,m))
r <- 0

sv <- ipop(c,H,A,b,l,u,r)
primal(sv)
dual(sv)
how(sv)</pre>
```

kcca

Kernel Canonical Correlation Analysis

# Description

Computes the canonical correlation analysis in feature space.

# Usage

```
## S4 method for signature 'matrix'
kcca(x, y, kernel="rbfdot", kpar=list(sigma=0.1),
gamma = 0.1, ncomps = 10, ...)
```

### **Arguments**

X

a matrix containing data index by row

У

a matrix containing data index by row

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a inner product in feature space between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function

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• splinedot Spline kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

gamma regularization parameter (default : 0.1)

ncomps number of canonical components (default : 10)
... additional parameters for the kpca function

#### **Details**

The kernel version of canonical correlation analysis. Kernel Canonical Correlation Analysis (KCCA) is a non-linear extension of CCA. Given two random variables, KCCA aims at extracting the information which is shared by the two random variables. More precisely given x and y the purpose of KCCA is to provide nonlinear mappings f(x) and g(y) such that their correlation is maximized.

#### Value

An S4 object containing the following slots:

kcor Correlation coefficients in feature space

xcoef estimated coefficients for the x variables in the feature space ycoef estimated coefficients for the y variables in the feature space

#### Author(s)

Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>

#### References

Malte Kuss, Thore Graepel

The Geometry Of Kernel Canonical Correlation Analysis

https://www.microsoft.com/en-us/research/publication/the-geometry-of-kernel-canonical-correlation-a

### See Also

cancor, kpca, kfa, kha

kcca-class 27

### **Examples**

```
## dummy data
x <- matrix(rnorm(30),15)
y <- matrix(rnorm(30),15)
kcca(x,y,ncomps=2)</pre>
```

kcca-class

Class "kcca"

# Description

The "kcca" class

# **Objects from the Class**

Objects can be created by calls of the form new("kcca", ...). or by the calling the kcca function.

### **Slots**

```
kcor: Object of class "vector" describing the correlations
xcoef: Object of class "matrix" estimated coefficients for the x variables
ycoef: Object of class "matrix" estimated coefficients for the y variables
```

### Methods

```
kcor signature(object = "kcca"): returns the correlations
xcoef signature(object = "kcca"): returns the estimated coefficients for the x variables
ycoef signature(object = "kcca"): returns the estimated coefficients for the y variables
```

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
kcca, kpca-class
```

```
## dummy data
x <- matrix(rnorm(30),15)
y <- matrix(rnorm(30),15)
kcca(x,y,ncomps=2)</pre>
```

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kernel-class

Class "kernel" "rbfkernel" "polykernel", "tanhkernel", "vanillakernel"

# Description

The built-in kernel classes in **kernlab** 

### **Objects from the Class**

```
Objects can be created by calls of the form new("rbfkernel"), new{"polykernel"}, new{"tanhkernel"}, new{"vanillakernel"}, new{"anovakernel"}, new{"besselkernel"}, new{"laplacekernel"}, new{"splinekernel"}, new{"stringkernel"}
```

or by calling the rbfdot, polydot, tanhdot, vanilladot, anovadot, besseldot, laplacedot, splinedot, stringdot functions etc..

#### Slots

```
.Data: Object of class "function" containing the kernel function kpar: Object of class "list" containing the kernel parameters
```

#### **Extends**

```
Class "kernel", directly. Class "function", by class "kernel".
```

#### Methods

```
kernelMatrix signature(kernel = "rbfkernel", x = "matrix"): computes the kernel matrix
kernelMult signature(kernel = "rbfkernel", x = "matrix"): computes the quadratic kernel
expression
```

```
kernelPol signature(kernel = "rbfkernel", x = "matrix"): computes the kernel expansion
```

**kernelFast** signature(kernel = "rbfkernel", x = "matrix"), a: computes parts or the full kernel matrix, mainly used in kernel algorithms where columns of the kernel matrix are computed per invocation

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

dots

kernelMatrix 29

### **Examples**

```
rbfkernel <- rbfdot(sigma = 0.1)
rbfkernel
is(rbfkernel)
kpar(rbfkernel)</pre>
```

kernelMatrix

Kernel Matrix functions

# Description

```
kernelMatrix calculates the kernel matrix K_{ij}=k(x_i,x_j) or K_{ij}=k(x_i,y_j). kernelPol computes the quadratic kernel expression H=z_iz_jk(x_i,x_j), H=z_ik_jk(x_i,y_j). kernelMult calculates the kernel expansion f(x_i)=\sum_{i=1}^m z_ik(x_i,x_j) kernelFast computes the kernel matrix, identical to kernelMatrix, except that it also requires the squared norm of the first argument as additional input, useful in iterative kernel matrix calculations.
```

# Usage

```
## S4 method for signature 'kernel'
kernelMatrix(kernel, x, y = NULL)

## S4 method for signature 'kernel'
kernelPol(kernel, x, y = NULL, z, k = NULL)

## S4 method for signature 'kernel'
kernelMult(kernel, x, y = NULL, z, blocksize = 256)

## S4 method for signature 'kernel'
kernelFast(kernel, x, y, a)
```

### **Arguments**

kernel	the kernel function to be used to calculate the kernel matrix. This has to be a function of class kernel, i.e. which can be generated either one of the build in kernel generating functions (e.g., rbfdot etc.) or a user defined function of class kernel taking two vector arguments and returning a scalar.
Х	a data matrix to be used to calculate the kernel matrix, or a list of vector when a stringkernel is used
У	second data matrix to calculate the kernel matrix, or a list of vector when a stringkernel is used
Z	a suitable vector or matrix
k	a suitable vector or matrix
а	the squared norm of x, e.g., rowSums( $x^2$ )

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blocksize

the kernel expansion computations are done block wise to avoid storing the kernel matrix into memory. blocksize defines the size of the computational blocks.

#### **Details**

Common functions used during kernel based computations.

The kernel parameter can be set to any function, of class kernel, which computes the inner product in feature space between two vector arguments. **kernlab** provides the most popular kernel functions which can be initialized by using the following functions:

- rbfdot Radial Basis kernel function
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot the Spline kernel

(see example.)

kernelFast is mainly used in situations where columns of the kernel matrix are computed per invocation. In these cases, evaluating the norm of each row-entry over and over again would cause significant computational overhead.

#### Value

kernelMatrix returns a symmetric diagonal semi-definite matrix. kernelPol returns a matrix. kernelMult usually returns a one-column matrix.

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
rbfdot, polydot, tanhdot, vanilladot
```

```
## use the spam data
data(spam)
dt <- as.matrix(spam[c(10:20,3000:3010),-58])
## initialize kernel function
rbf <- rbfdot(sigma = 0.05)</pre>
```

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```
## calculate kernel matrix
kernelMatrix(rbf, dt)

yt <- as.matrix(as.integer(spam[c(10:20,3000:3010),58]))
yt[yt==2] <- -1

## calculate the quadratic kernel expression
kernelPol(rbf, dt, ,yt)

## calculate the kernel expansion
kernelMult(rbf, dt, ,yt)</pre>
```

kfa

Kernel Feature Analysis

# Description

The Kernel Feature Analysis algorithm is an algorithm for extracting structure from possibly highdimensional data sets. Similar to kpca a new basis for the data is found. The data can then be projected on the new basis.

#### Usage

```
## S4 method for signature 'formula'
kfa(x, data = NULL, na.action = na.omit, ...)
## S4 method for signature 'matrix'
kfa(x, kernel = "rbfdot", kpar = list(sigma = 0.1),
    features = 0, subset = 59, normalize = TRUE, na.action = na.omit)
```

### **Arguments**

Х

The data matrix indexed by row or a formula describing the model. Note, that an intercept is always included, whether given in the formula or not.

data

an optional data frame containing the variables in the model (when using a formula).

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes an inner product in feature space between two vector arguments. **kernlab** provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function

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- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- · anovadot ANOVA RBF kernel function
- splinedot Spline kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

features Number of features (principal components) to return. (default: 0, all)

subset the number of features sampled (used) from the data set

normalize normalize the feature selected (default: TRUE)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

... additional parameters

#### **Details**

Kernel Feature analysis is similar to Kernel PCA, but instead of extracting eigenvectors of the training dataset in feature space, it approximates the eigenvectors by selecting training patterns which are good basis vectors for the training set. It works by choosing a fixed size subset of the data set and scaling it to unit length (under the kernel). It then chooses the features that maximize the value of the inner product (kernel function) with the rest of the patterns.

#### Value

kfa returns an object of class kfa containing the features selected by the algorithm.

xmatrix contains the features selected alpha contains the sparse alpha vector

The predict function can be used to embed new data points into to the selected feature base.

#### Author(s)

Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>

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#### References

```
Alex J. Smola, Olvi L. Mangasarian and Bernhard Schoelkopf 
Sparse Kernel Feature Analysis
Data Mining Institute Technical Report 99-04, October 1999
ftp://ftp.cs.wisc.edu/pub/dmi/tech-reports/99-04.ps
```

#### See Also

```
kpca, kfa-class
```

### **Examples**

kfa-class

Class "kfa"

### **Description**

The class of the object returned by the Kernel Feature Analysis kfa function

### **Objects from the Class**

Objects can be created by calls of the form new("kfa", ...) or by calling the kfa method. The objects contain the features along with the alpha values.

# Slots

```
alpha: Object of class "matrix" containing the alpha values alphaindex: Object of class "vector" containing the indexes of the selected feature kernelf: Object of class "kfunction" containing the kernel function used xmatrix: Object of class "matrix" containing the selected features kcall: Object of class "call" containing the kfa function call terms: Object of class "ANY" containing the formula terms
```

### Methods

```
alpha signature(object = "kfa"): returns the alpha values
alphaindex signature(object = "kfa"): returns the index of the selected features
kcall signature(object = "kfa"): returns the function call
kernelf signature(object = "kfa"): returns the kernel function used
predict signature(object = "kfa"): used to embed more data points to the feature base
xmatrix signature(object = "kfa"): returns the selected features.
```

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#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
kfa, kpca-class
```

### **Examples**

```
data(promotergene)
f <- kfa(~.,data=promotergene)</pre>
```

kha

Kernel Principal Components Analysis

# Description

Kernel Hebbian Algorithm is a nonlinear iterative algorithm for principal component analysis.

# Usage

# **Arguments**

Χ

The data matrix indexed by row or a formula describing the model. Note, that an intercept is always included, whether given in the formula or not.

data

an optional data frame containing the variables in the model (when using a formula).

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes the inner product in feature space between two vector arguments (see kernels). **kernlab** provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function

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- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

features Number of features (principal components) to return. (default: 5)

eta The hebbian learning rate (default : 0.005)

th the smallest value of the convergence step (default : 0.0001)

maxiter the maximum number of iterations.

verbose print convergence every 100 iterations. (default : FALSE)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

... additional parameters

#### **Details**

The original form of KPCA can only be used on small data sets since it requires the estimation of the eigenvectors of a full kernel matrix. The Kernel Hebbian Algorithm iteratively estimates the Kernel Principal Components with only linear order memory complexity. (see ref. for more details)

#### Value

An S4 object containing the principal component vectors along with the corresponding normalization values.

pcv a matrix containing the principal component vectors (column wise)

eig The normalization values xmatrix The original data matrix

all the slots of the object can be accessed by accessor functions.

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### Note

The predict function can be used to embed new data on the new space

# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### References

```
Kwang In Kim, M.O. Franz and B. Schölkopf

Kernel Hebbian Algorithm for Iterative Kernel Principal Component Analysis

Max-Planck-Institut für biologische Kybernetik, Tübingen (109)

https://is.mpg.de/fileadmin/user_upload/files/publications/pdf2302.pdf
```

#### See Also

```
kpca, kfa, kcca, pca
```

### **Examples**

kha-class

Class "kha"

### **Description**

The Kernel Hebbian Algorithm class

# Objects objects of class "kha"

Objects can be created by calls of the form new("kha", ...). or by calling the kha function.

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## Slots

```
pcv: Object of class "matrix" containing the principal component vectors eig: Object of class "vector" containing the corresponding normalization values eskm: Object of class "vector" containing the kernel sum kernelf: Object of class "kfunction" containing the kernel function used kpar: Object of class "list" containing the kernel parameters used xmatrix: Object of class "matrix" containing the data matrix used kcall: Object of class "ANY" containing the function call n.action: Object of class "ANY" containing the action performed on NA
```

## Methods

```
eig signature(object = "kha"): returns the normalization values
kcall signature(object = "kha"): returns the performed call
kernelf signature(object = "kha"): returns the used kernel function
pcv signature(object = "kha"): returns the principal component vectors
eskm signature(object = "kha"): returns the kernel sum
predict signature(object = "kha"): embeds new data
xmatrix signature(object = "kha"): returns the used data matrix
```

# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

# See Also

```
kha, ksvm-class, kcca-class
```

# **Examples**

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kkmeans

Kernel k-means

# Description

A weighted kernel version of the famous k-means algorithm.

## Usage

### **Arguments**

х

the matrix of data to be clustered, or a symbolic description of the model to be fit, or a kernel Matrix of class kernelMatrix, or a list of character vectors.

data

an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'kkmeans' is called from.

centers

Either the number of clusters or a matrix of initial cluster centers. If the first a random initial partitioning is used.

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a inner product in feature space between two vector arguments (see link{kernels}). **kernlab** provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel "Gaussian"
- polydot Polynomial kernel
- vanilladot Linear kernel
- tanhdot Hyperbolic tangent kernel
- laplacedot Laplacian kernel
- besseldot Bessel kernel
- anovadot ANOVA RBF kernel
- splinedot Spline kernel

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• stringdot String kernel

Setting the kernel parameter to "matrix" treats x as a kernel matrix calling the kernelMatrix interface.

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

a character string or the list of hyper-parameters (kernel parameters). The default character string "automatic" uses a heuristic the determine a suitable value for the width parameter of the RBF kernel.

A list can also be used containing the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".
- length, lambda, normalized for the "stringdot" kernel where length is
  the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be
  normalized.

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

alg the algorithm to use. Options currently include kkmeans and kerninghan.

p a parameter used to keep the affinity matrix positive semidefinite

na.action The action to perform on NA

... additional parameters

#### **Details**

kernel k-means uses the 'kernel trick' (i.e. implicitly projecting all data into a non-linear feature space with the use of a kernel) in order to deal with one of the major drawbacks of k-means that is that it cannot capture clusters that are not linearly separable in input space.

The algorithm is implemented using the triangle inequality to avoid unnecessary and computational expensive distance calculations. This leads to significant speedup particularly on large data sets with a high number of clusters.

With a particular choice of weights this algorithm becomes equivalent to Kernighan-Lin, and the norm-cut graph partitioning algorithms.

The function also support input in the form of a kernel matrix or a list of characters for text clustering.

The data can be passed to the kkmeans function in a matrix or a data.frame, in addition kkmeans also supports input in the form of a kernel matrix of class kernelMatrix or as a list of character vectors where a string kernel has to be used.

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## Value

An S4 object of class specc which extends the class vector containing integers indicating the cluster to which each point is allocated. The following slots contain useful information

centers A matrix of cluster centers.

size The number of point in each cluster

withinss The within-cluster sum of squares for each cluster

kernelf The kernel function used

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### References

```
Inderjit Dhillon, Yuqiang Guan, Brian Kulis
A Unified view of Kernel k-means, Spectral Clustering and Graph Partitioning
UTCS Technical Report
https://people.bu.edu/bkulis/pubs/spectral_techreport.pdf
```

#### See Also

```
specc, kpca, kcca
```

# **Examples**

```
## Cluster the iris data set.
data(iris)
sc <- kkmeans(as.matrix(iris[,-5]), centers=3)
sc
centers(sc)
size(sc)
withinss(sc)</pre>
```

kmmd

Kernel Maximum Mean Discrepancy.

# **Description**

The Kernel Maximum Mean Discrepancy kmmd performs a non-parametric distribution test.

kmmd 41

## Usage

### **Arguments**

x data values, in a matrix, list, or kernelMatrix

y data values, in a matrix, list, or kernelMatrix

Kxy kernlMatrix between x and y values (only for the kernelMatrix interface)

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel
- stringdot String kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

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lenght, lambda, normalized for the "stringdot" kernel where length is
the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be
normalized.

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well. In the case of a Radial Basis kernel function (Gaussian) kpar can also be set to the string "automatic" which uses the heuristics in 'sigest' to calculate a good 'sigma' value for the Gaussian RBF or Laplace kernel, from the data. (default = "automatic").

the data. (default – automatic ).

alpha the confidence level of the test (default: 0.05)

asymptotic calculate the bounds asymptotically (suitable for smaller datasets) (default: FALSE) replace use replace when sampling for computing the asymptotic bounds (default: TRUE)

ntimes number of times repeating the sampling procedure (default : 150)

frac fraction of points to sample (frac : 1)

... additional parameters.

#### **Details**

kmmd calculates the kernel maximum mean discrepancy for samples from two distributions and conducts a test as to whether the samples are from different distributions with level alpha.

### Value

An S4 object of class kmmd containing the results of whether the H0 hypothesis is rejected or not. H0 being that the samples x and y come from the same distribution. The object contains the following slots:

H0 is H0 rejected (logical)

AsympH0 is H0 rejected according to the asymptotic bound (logical)

kernelf the kernel function used.

mmdstats the test statistics (vector of two)

Radbound the Rademacher bound Asymbound the asymptotic bound

see kmmd-class for more details.

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### References

```
Gretton, A., K. Borgwardt, M. Rasch, B. Schoelkopf and A. Smola 
A Kernel Method for the Two-Sample-Problem

Neural Information Processing Systems 2006, Vancouver

https://papers.neurips.cc/paper/3110-a-kernel-method-for-the-two-sample-problem.

pdf
```

kmmd-class 43

## See Also

ksvm

### **Examples**

```
# create data
x <- matrix(runif(300),100)
y <- matrix(runif(300)+1,100)

mmdo <- kmmd(x, y)

mmdo</pre>
```

kmmd-class

Class "kqr"

# **Description**

The Kernel Maximum Mean Discrepancy object class

## **Objects from the Class**

Objects can be created by calls of the form new("kmmd", ...). or by calling the kmmd function

## **Slots**

```
kernelf: Object of class "kfunction" contains the kernel function used
xmatrix: Object of class "kernelMatrix" containing the data used
H0 Object of class "logical" contains value of: is H0 rejected (logical)
AsympH0 Object of class "logical" contains value: is H0 rejected according to the asymptotic bound (logical)
mmdstats Object of class "vector" contains the test statistics (vector of two)
Radbound Object of class "numeric" contains the Rademacher bound
Asymbound Object of class "numeric" contains the asymptotic bound
```

# Methods

```
kernelf signature(object = "kmmd"): returns the kernel function used
H0 signature(object = "kmmd"): returns the value of H0 being rejected
AsympH0 signature(object = "kmmd"): returns the value of H0 being rejected according to the
    asymptotic bound
mmdstats signature(object = "kmmd"): returns the values of the mmd statistics
Radbound signature(object = "kmmd"): returns the value of the Rademacher bound
Asymbound signature(object = "kmmd"): returns the value of the asymptotic bound
```

kpca kpca

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### See Also

kmmd,

# **Examples**

```
# create data
x <- matrix(runif(300),100)
y <- matrix(runif(300)+1,100)

mmdo <- kmmd(x, y)

H0(mmdo)</pre>
```

kpca

Kernel Principal Components Analysis

# **Description**

Kernel Principal Components Analysis is a nonlinear form of principal component analysis.

# Usage

```
## S4 method for signature 'formula'
kpca(x, data = NULL, na.action, ...)

## S4 method for signature 'matrix'
kpca(x, kernel = "rbfdot", kpar = list(sigma = 0.1),
    features = 0, th = 1e-4, na.action = na.omit, ...)

## S4 method for signature 'kernelMatrix'
kpca(x, features = 0, th = 1e-4, ...)

## S4 method for signature 'list'
kpca(x, kernel = "stringdot", kpar = list(length = 4, lambda = 0.5),
    features = 0, th = 1e-4, na.action = na.omit, ...)
```

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### **Arguments**

Х

the data matrix indexed by row or a formula describing the model, or a kernel Matrix of class kernelMatrix, or a list of character vectors

data

an optional data frame containing the variables in the model (when using a formula).

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

features

Number of features (principal components) to return. (default: 0, all)

th

the value of the eigenvalue under which principal components are ignored (only valid when features = 0). (default : 0.0001)

na.action

A function to specify the action to be taken if NAs are found. The default action is na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found. (NOTE: If given, this argument must be named.)

... additional parameters

# Details

Using kernel functions one can efficiently compute principal components in high-dimensional feature spaces, related to input space by some non-linear map.

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The data can be passed to the kpca function in a matrix or a data. frame, in addition kpca also supports input in the form of a kernel matrix of class kernelMatrix or as a list of character vectors where a string kernel has to be used.

### Value

An S4 object containing the principal component vectors along with the corresponding eigenvalues.

pcv a matrix containing the principal component vectors (column wise)

eig The corresponding eigenvalues

rotated The original data projected (rotated) on the principal components

xmatrix The original data matrix

all the slots of the object can be accessed by accessor functions.

### Note

The predict function can be used to embed new data on the new space

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### References

```
Schoelkopf B., A. Smola, K.-R. Mueller: Nonlinear component analysis as a kernel eigenvalue problem Neural Computation 10, 1299-1319 doi:10.1162/089976698300017467.
```

# See Also

```
kcca, pca
```

## **Examples**

kpca-class 47

```
#embed remaining points
emb <- predict(kpc,iris[test,-5])
points(emb,col=as.integer(iris[test,5]))</pre>
```

kpca-class

Class "kpca"

### **Description**

The Kernel Principal Components Analysis class

# Objects of class "kpca"

Objects can be created by calls of the form new("kpca", ...). or by calling the kpca function.

### **Slots**

```
pcv: Object of class "matrix" containing the principal component vectors
eig: Object of class "vector" containing the corresponding eigenvalues
rotated: Object of class "matrix" containing the projection of the data on the principal components
kernelf: Object of class "function" containing the kernel function used
kpar: Object of class "list" containing the kernel parameters used
xmatrix: Object of class "matrix" containing the data matrix used
kcall: Object of class "ANY" containing the function call
n.action: Object of class "ANY" containing the action performed on NA
```

### Methods

```
eig signature(object = "kpca"): returns the eigenvalues
kcall signature(object = "kpca"): returns the performed call
kernelf signature(object = "kpca"): returns the used kernel function
pcv signature(object = "kpca"): returns the principal component vectors
predict signature(object = "kpca"): embeds new data
rotated signature(object = "kpca"): returns the projected data
xmatrix signature(object = "kpca"): returns the used data matrix
```

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

## See Also

```
ksvm-class, kcca-class
```

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## **Examples**

kqr

Kernel Quantile Regression.

# Description

The Kernel Quantile Regression algorithm kqr performs non-parametric Quantile Regression.

# Usage

# Arguments

Х

e data or a symbolic description of the model to be fit. When not using a formula x can be a matrix or vector containing the training data or a kernel matrix of class kernelMatrix of the training data or a list of character vectors (for use with the string kernel). Note, that the intercept is always excluded, whether given in the formula or not.

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data

an optional data frame containing the variables in the model. By default the variables are taken from the environment which kqr is called from.

У

a numeric vector or a column matrix containing the response.

scaled

A logical vector indicating the variables to be scaled. If scaled is of length 1, the value is recycled as many times as needed and all non-binary variables are scaled. Per default, data are scaled internally (both x and y variables) to zero mean and unit variance. The center and scale values are returned and used for later predictions. (default: TRUE)

tau

the quantile to be estimated, this is generally a number strictly between 0 and 1. For 0.5 the median is calculated. (default: 0.5)

С

the cost regularization parameter. This parameter controls the smoothness of the fitted function, essentially higher values for C lead to less smooth functions.(default: 1)

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel
- stringdot String kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. Valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".
- lenght, lambda, normalized for the "stringdot" kernel where length is
  the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be
  normalized.

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well. In the case of a Radial Basis kernel function (Gaussian) kpar

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can also be set to the string "automatic" which uses the heuristics in 'sigest' to calculate a good 'sigma' value for the Gaussian RBF or Laplace kernel, from

the data. (default = "automatic").

reduced use an incomplete cholesky decomposition to calculate a decomposed form Z

of the kernel Matrix K (where K = ZZ') and perform the calculations with Z. This might be useful when using kqr with large datasets since normally an n times n kernel matrix would be computed. Setting reduced to TRUE makes use of csi to compute a decomposed form instead and thus only a  $n \times m$  matrix where m < n and n the sample size is stored in memory (default: FALSE)

rank the rank m of the decomposed matrix calculated when using an incomplete

cholesky decomposition. This parameter is only taken into account when reduced

is TRUE(default : dim(x)[1]/6)

fit indicates whether the fitted values should be computed and included in the

model or not (default: 'TRUE')

cross if a integer value k>0 is specified, a k-fold cross validation on the training data is

performed to assess the quality of the model: the Pinball loss and the for quantile

regression

subset An index vector specifying the cases to be used in the training sample. (NOTE:

If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

... additional parameters.

### **Details**

In quantile regression a function is fitted to the data so that it satisfies the property that a portion tau of the data y|n is below the estimate. While the error bars of many regression problems can be viewed as such estimates quantile regression estimates this quantity directly. Kernel quantile regression is similar to nu-Support Vector Regression in that it minimizes a regularized loss function in RKHS. The difference between nu-SVR and kernel quantile regression is in the type of loss function used which in the case of quantile regression is the pinball loss (see reference for details.). Minimizing the regularized loss boils down to a quadratic problem which is solved using an interior point QP solver ipop implemented in kernlab.

#### Value

An S4 object of class kqr containing the fitted model along with information. Accessor functions can be used to access the slots of the object which include:

alpha The resulting model parameters which can be also accessed by coef.

kernelf the kernel function used.

error Training error (if fit == TRUE)

see kqr-class for more details.

kqr-class 51

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### References

```
Ichiro Takeuchi, Quoc V. Le, Timothy D. Sears, Alexander J. Smola 
Nonparametric Quantile Estimation

Journal of Machine Learning Research 7,2006,1231-1264

https://www.jmlr.org/papers/volume7/takeuchi06a/takeuchi06a.pdf
```

### See Also

```
predict.kqr, kqr-class, ipop, rvm, ksvm
```

# **Examples**

```
# create data
x \leftarrow sort(runif(300))
y \leftarrow sin(pi*x) + rnorm(300,0,sd=exp(sin(2*pi*x)))
# first calculate the median
qrm <- kqr(x, y, tau = 0.5, C=0.15)
# predict and plot
plot(x, y)
ytest <- predict(qrm, x)</pre>
lines(x, ytest, col="blue")
# calculate 0.9 quantile
qrm \leftarrow kqr(x, y, tau = 0.9, kernel = "rbfdot",
            kpar= list(sigma=10), C=0.15)
ytest <- predict(qrm, x)</pre>
lines(x, ytest, col="red")
# calculate 0.1 quantile
qrm <- kqr(x, y, tau = 0.1,C=0.15)
ytest <- predict(qrm, x)</pre>
lines(x, ytest, col="green")
# print first 10 model coefficients
coef(qrm)[1:10]
```

kqr-class

Class "kqr"

# **Description**

The Kernel Quantile Regression object class

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## **Objects from the Class**

Objects can be created by calls of the form new("kqr", ...). or by calling the kqr function

### **Slots**

```
kernelf: Object of class "kfunction" contains the kernel function used
kpar: Object of class "list" contains the kernel parameter used
coef: Object of class "ANY" containing the model parameters
param: Object of class "list" contains the cost parameter C and tau parameter used
kcall: Object of class "list" contains the used function call
terms: Object of class "ANY" contains the terms representation of the symbolic model used (when
     using a formula)
xmatrix: Object of class "input" containing the data matrix used
ymatrix: Object of class "output" containing the response matrix
fitted: Object of class "output" containing the fitted values
alpha: Object of class "listI" containing the computes alpha values
b: Object of class "numeric" containing the offset of the model.
scaling Object of class "ANY" containing the scaling coefficients of the data (when case scaled =
     TRUE is used).
error: Object of class "numeric" containing the training error
cross: Object of class "numeric" containing the cross validation error
n.action: Object of class "ANY" containing the action performed in NA
nclass: Inherited from class vm, not used in kgr
lev: Inherited from class vm, not used in kgr
type: Inherited from class vm, not used in kgr
```

### Methods

```
coef signature(object = "kqr"): returns the coefficients (alpha) of the model
alpha signature(object = "kqr"): returns the alpha vector (identical to coef)
b signature(object = "kqr"): returns the offset beta of the model.
cross signature(object = "kqr"): returns the cross validation error
error signature(object = "kqr"): returns the training error
fitted signature(object = "vm"): returns the fitted values
kcall signature(object = "kqr"): returns the call performed
kernelf signature(object = "kqr"): returns the kernel function used
kpar signature(object = "kqr"): returns the kernel parameter used
param signature(object = "kqr"): returns the cost regularization parameter C and tau used
xmatrix signature(object = "kqr"): returns the data matrix used
ymatrix signature(object = "kqr"): returns the response matrix used
scaling signature(object = "kqr"): returns the scaling coefficients of the data (when scaled =
TRUE is used)
```

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### See Also

```
kgr, vm-class, ksvm-class
```

# **Examples**

```
# create data
x \leftarrow sort(runif(300))
y \leftarrow sin(pi*x) + rnorm(300,0,sd=exp(sin(2*pi*x)))
# first calculate the median
qrm <- kqr(x, y, tau = 0.5, C=0.15)
# predict and plot
plot(x, y)
ytest <- predict(qrm, x)</pre>
lines(x, ytest, col="blue")
# calculate 0.9 quantile
qrm \leftarrow kqr(x, y, tau = 0.9, kernel = "rbfdot",
            kpar = list(sigma = 10), C = 0.15)
ytest <- predict(qrm, x)</pre>
lines(x, ytest, col="red")
# print model coefficients and other information
coef(qrm)
b(qrm)
error(qrm)
kernelf(qrm)
```

ksvm

Support Vector Machines

# Description

Support Vector Machines are an excellent tool for classification, novelty detection, and regression. ksvm supports the well known C-svc, nu-svc, (classification) one-class-svc (novelty) eps-svr, nu-svr (regression) formulations along with native multi-class classification formulations and the bound-constraint SVM formulations.

ksvm also supports class-probabilities output and confidence intervals for regression.

### **Usage**

```
## S4 method for signature 'formula'
ksvm(x, data = NULL, ..., subset, na.action = na.omit, scaled = TRUE)
## S4 method for signature 'vector'
ksvm(x, ...)
## S4 method for signature 'matrix'
ksvm(x, y = NULL, scaled = TRUE, type = NULL,
     kernel ="rbfdot", kpar = "automatic",
     C = 1, nu = 0.2, epsilon = 0.1, prob.model = FALSE,
     class.weights = NULL, cross = 0, fit = TRUE, cache = 40,
     tol = 0.001, shrinking = TRUE, ...,
     subset, na.action = na.omit)
## S4 method for signature 'kernelMatrix'
ksvm(x, y = NULL, type = NULL,
     C = 1, nu = 0.2, epsilon = 0.1, prob.model = FALSE,
     class.weights = NULL, cross = 0, fit = TRUE, cache = 40,
     tol = 0.001, shrinking = TRUE, ...)
## S4 method for signature 'list'
ksvm(x, y = NULL, type = NULL,
     kernel = "stringdot", kpar = list(length = 4, lambda = 0.5),
     C = 1, nu = 0.2, epsilon = 0.1, prob.model = FALSE,
     class.weights = NULL, cross = 0, fit = TRUE, cache = 40,
     tol = 0.001, shrinking = TRUE, ...,
     na.action = na.omit)
```

## Arguments

x

a symbolic description of the model to be fit. When not using a formula x can be a matrix or vector containing the training data or a kernel matrix of class kernelMatrix of the training data or a list of character vectors (for use with the string kernel). Note, that the intercept is always excluded, whether given in the formula or not.

data

an optional data frame containing the training data, when using a formula. By default the data is taken from the environment which 'ksvm' is called from.

У

a response vector with one label for each row/component of x. Can be either a factor (for classification tasks) or a numeric vector (for regression).

scaled

A logical vector indicating the variables to be scaled. If scaled is of length 1, the value is recycled as many times as needed and all non-binary variables are scaled. Per default, data are scaled internally (both x and y variables) to zero mean and unit variance. The center and scale values are returned and used for later predictions.

type

ksvm can be used for classification, for regression, or for novelty detection. Depending on whether y is a factor or not, the default setting for type is C-svc or eps-svr, respectively, but can be overwritten by setting an explicit value. Valid options are:

- C-svc C classification
- nu-svc nu classification
- C-bsvc bound-constraint svm classification
- spoc-svc Crammer, Singer native multi-class
- kbb-svc Weston, Watkins native multi-class
- one-svc novelty detection
- eps-svr epsilon regression
- nu-svr nu regression
- eps-bsvr bound-constraint svm regression

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes the inner product in feature space between two vector arguments (see kernels).

kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel "Gaussian"
- polydot Polynomial kernel
- vanilladot Linear kernel
- tanhdot Hyperbolic tangent kernel
- laplacedot Laplacian kernel
- besseldot Bessel kernel
- anovadot ANOVA RBF kernel
- splinedot Spline kernel
- stringdot String kernel

kernels are:

Setting the kernel parameter to "matrix" treats x as a kernel matrix calling the kernelMatrix interface.

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. For valid parameters for existing

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".
- length, lambda, normalized for the "stringdot" kernel where length is the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be normalized.

iter ner

kpar

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well. In the case of a Radial Basis kernel function (Gaussian) kpar can also be set to the string "automatic" which uses the heuristics in sigest to calculate a good sigma value for the Gaussian RBF or Laplace kernel, from the data. (default = "automatic").

cost of constraints violation (default: 1) this is the 'C'-constant of the regular-

ization term in the Lagrange formulation.

nu parameter needed for nu-svc, one-svc, and nu-svr. The nu parameter sets the

upper bound on the training error and the lower bound on the fraction of data

points to become Support Vectors (default: 0.2).

epsilon epsilon in the insensitive-loss function used for eps-svr, nu-svr and eps-bsvm

(default: 0.1)

prob.model if set to TRUE builds a model for calculating class probabilities or in case of

regression, calculates the scaling parameter of the Laplacian distribution fitted on the residuals. Fitting is done on output data created by performing a 3-fold cross-validation on the training data. For details see references. (default: FALSE)

class.weights a named vector of weights for the different classes, used for asymmetric class

sizes. Not all factor levels have to be supplied (default weight: 1). All compo-

nents have to be named.

cache cache memory in MB (default 40)

tol tolerance of termination criterion (default: 0.001)

shrinking option whether to use the shrinking-heuristics (default: TRUE)

cross if a integer value k>0 is specified, a k-fold cross validation on the training data is

performed to assess the quality of the model: the accuracy rate for classification

and the Mean Squared Error for regression

fit indicates whether the fitted values should be computed and included in the

model or not (default: TRUE)

... additional parameters for the low level fitting function

subset An index vector specifying the cases to be used in the training sample. (NOTE:

If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

# **Details**

С

ksvm uses John Platt's SMO algorithm for solving the SVM QP problem an most SVM formulations. On the spoc-svc, kbb-svc, C-bsvc and eps-bsvr formulations a chunking algorithm based on the TRON QP solver is used.

For multiclass-classification with k classes, k>2, ksvm uses the 'one-against-one'-approach, in which k(k-1)/2 binary classifiers are trained; the appropriate class is found by a voting scheme, The spoc-svc and the kbb-svc formulations deal with the multiclass-classification problems by solving a single quadratic problem involving all the classes.

If the predictor variables include factors, the formula interface must be used to get a correct model

matrix.

In classification when prob. model is TRUE a 3-fold cross validation is performed on the data and a sigmoid function is fitted on the resulting decision values f. The data can be passed to the ksvm function in a matrix or a data. frame, in addition ksvm also supports input in the form of a kernel matrix of class kernelMatrix or as a list of character vectors where a string kernel has to be used. The plot function for binary classification ksvm objects displays a contour plot of the decision values with the corresponding support vectors highlighted.

The predict function can return class probabilities for classification problems by setting the type parameter to "probabilities".

The problem of model selection is partially addressed by an empirical observation for the RBF kernels (Gaussian , Laplace) where the optimal values of the sigma width parameter are shown to lie in between the 0.1 and 0.9 quantile of the  $\|x-x'\|$  statistics. When using an RBF kernel and setting kpar to "automatic", ksvm uses the sigest function to estimate the quantiles and uses the median of the values.

### Value

An S4 object of class "ksvm" containing the fitted model, Accessor functions can be used to access the slots of the object (see examples) which include:

alpha The resulting support vectors, (alpha vector) (possibly scaled).

alphaindex The index of the resulting support vectors in the data matrix. Note that this

index refers to the pre-processed data (after the possible effect of na.omit and

subset)

coef The corresponding coefficients times the training labels.

b The negative intercept.

nSV The number of Support Vectors

obj The value of the objective function. In case of one-against-one classification this

is a vector of values

error Training error

cross Cross validation error, (when cross > 0)

prob.model Contains the width of the Laplacian fitted on the residuals in case of regres-

sion, or the parameters of the sigmoid fitted on the decision values in case of

classification.

# Note

Data is scaled internally by default, usually yielding better results.

## Author(s)

Alexandros Karatzoglou (SMO optimizers in C++ by Chih-Chung Chang & Chih-Jen Lin) <alexandros.karatzoglou@ci.tuwien.ac.at>

### References

Chang Chih-Chung, Lin Chih-Jen
 LIBSVM: a library for Support Vector Machines
 https://www.csie.ntu.edu.tw/~cjlin/libsvm/

• Chih-Wei Hsu, Chih-Jen Lin

BSVM https://www.csie.ntu.edu.tw/~cjlin/bsvm/

• J. Platt

Probabilistic outputs for support vector machines and comparison to regularized likelihood methods

Advances in Large Margin Classifiers, A. Smola, P. Bartlett, B. Schoelkopf and D. Schuurmans, Eds. Cambridge, MA: MIT Press, 2000.

H.-T. Lin, C.-J. Lin and R. C. Weng
 A note on Platt's probabilistic outputs for support vector machines
 https://www.csie.ntu.edu.tw/~htlin/paper/doc/plattprob.pdf

· C.-W. Hsu and C.-J. Lin

A comparison on methods for multi-class support vector machines IEEE Transactions on Neural Networks, 13(2002) 415-425. https://www.csie.ntu.edu.tw/~cjlin/papers/multisvm.pdf

• K. Crammer, Y. Singer

On the learnability and design of output codes for multiclass prolems Computational Learning Theory, 35-46, 2000.

http://www.learningtheory.org/colt2000/papers/CrammerSinger.pdf

• J. Weston, C. Watkins

*Multi-class support vector machines*. Technical Report CSD-TR-98-04, Royal Holloway, University of London, Department of Computer Science.

#### See Also

```
predict.ksvm, ksvm-class, couple
```

## **Examples**

```
## Check results
table(mailtype,spamtest[,58])
## Another example with the famous iris data
data(iris)
## Create a kernel function using the build in rbfdot function
rbf <- rbfdot(sigma=0.1)</pre>
rbf
## train a bound constraint support vector machine
irismodel <- ksvm(Species~.,data=iris,type="C-bsvc",</pre>
                   kernel=rbf,C=10,prob.model=TRUE)
irismodel
## get fitted values
fitted(irismodel)
## Test on the training set with probabilities as output
predict(irismodel, iris[,-5], type="probabilities")
## Demo of the plot function
x <- rbind(matrix(rnorm(120),,2),matrix(rnorm(120,mean=3),,2))</pre>
y \leftarrow matrix(c(rep(1,60),rep(-1,60)))
svp <- ksvm(x,y,type="C-svc")</pre>
plot(svp,data=x)
### Use kernelMatrix
K <- as.kernelMatrix(crossprod(t(x)))</pre>
svp2 <- ksvm(K, y, type="C-svc")</pre>
svp2
# test data
xtest <- rbind(matrix(rnorm(20),,2),matrix(rnorm(20,mean=3),,2))</pre>
# test kernel matrix i.e. inner/kernel product of test data with
# Support Vectors
Ktest <- as.kernelMatrix(crossprod(t(xtest),t(x[SVindex(svp2), ])))</pre>
predict(svp2, Ktest)
#### Use custom kernel
k \leftarrow function(x,y) \{(sum(x*y) +1)*exp(-0.001*sum((x-y)^2))\}
class(k) <- "kernel"</pre>
```

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```
data(promotergene)
## train svm using custom kernel
gene <- ksvm(Class~.,data=promotergene[c(1:20, 80:100),],kernel=k,</pre>
             C=5, cross=5)
gene
#### Use text with string kernels
data(reuters)
is(reuters)
tsv <- ksvm(reuters,rlabels,kernel="stringdot",</pre>
            kpar=list(length=5),cross=3,C=10)
tsv
## regression
# create data
x < - seq(-20, 20, 0.1)
y <- \sin(x)/x + rnorm(401, sd=0.03)
# train support vector machine
regm <- ksvm(x,y,epsilon=0.01,kpar=list(sigma=16),cross=3)</pre>
plot(x,y,type="l")
lines(x,predict(regm,x),col="red")
```

ksvm-class

Class "ksvm"

## **Description**

An S4 class containing the output (model) of the ksvm Support Vector Machines function

# **Objects from the Class**

Objects can be created by calls of the form new("ksvm", ...) or by calls to the ksvm function.

# **Slots**

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```
terms: Object of class "ANY" containing the terms representation of the symbolic model used
         (when using a formula)
    xmatrix: Object of class "input" ("list" for multiclass problems or "matrix" for binary clas-
         sification and regression problems) containing the support vectors calculated from the data
         matrix used during computations (possibly scaled and without NA). In the case of multi-class
         classification each list entry contains the support vectors from each binary classification prob-
         lem from the one-against-one method.
    ymatrix: Object of class "output" the response "matrix" or "factor" or "vector" or "logical"
    fitted: Object of class "output" with the fitted values, predictions using the training set.
    lev: Object of class "vector" with the levels of the response (in the case of classification)
    prob.model: Object of class "list" with the class prob. model
    prior: Object of class "list" with the prior of the training set
    nclass: Object of class "numeric" containing the number of classes (in the case of classification)
    alpha: Object of class "listI" containing the resulting alpha vector ("list" or "matrix" in case
         of multiclass classification) (support vectors)
    coef: Object of class "ANY" containing the resulting coefficients
    alphaindex: Object of class "list" containing
    b: Object of class "numeric" containing the resulting offset
    SVindex: Object of class "vector" containing the indexes of the support vectors
    nSV: Object of class "numeric" containing the number of support vectors
    obj: Object of class vector containing the value of the objective function. When using one-
         against-one in multiclass classification this is a vector.
    error: Object of class "numeric" containing the training error
    cross: Object of class "numeric" containing the cross-validation error
    n.action: Object of class "ANY" containing the action performed for NA
Methods
    SVindex signature(object = "ksvm"): return the indexes of support vectors
    alpha signature(object = "ksvm"): returns the complete 5 alpha vector (wit zero values)
    alphaindex signature(object = "ksvm"): returns the indexes of non-zero alphas (support vec-
         tors)
    cross signature(object = "ksvm"): returns the cross-validation error
    error signature(object = "ksvm"): returns the training error
    obj signature(object = "ksvm"): returns the value of the objective function
    fitted signature(object = "vm"): returns the fitted values (predict on training set)
    kernelf signature(object = "ksvm"): returns the kernel function
    kpar signature(object = "ksvm"): returns the kernel parameters (hyperparameters)
    lev signature(object = "ksvm"): returns the levels in case of classification
    prob.model signature(object="ksvm"): returns class prob. model values
```

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```
param signature(object="ksvm"): returns the parameters of the SVM in a list (C, epsilon, nu etc.)

prior signature(object="ksvm"): returns the prior of the training set

kcall signature(object="ksvm"): returns the ksvm function call

scaling signature(object = "ksvm"): returns the scaling values

show signature(object = "ksvm"): prints the object information

type signature(object = "ksvm"): returns the problem type

xmatrix signature(object = "ksvm"): returns the data matrix used

ymatrix signature(object = "ksvm"): returns the response vector
```

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzolgou@ci.tuwien.ac.at>
```

## See Also

```
ksvm, rvm-class, gausspr-class
```

# **Examples**

```
## simple example using the promotergene data set
data(promotergene)
## train a support vector machine
gene <- ksvm(Class~.,data=promotergene,kernel="rbfdot",</pre>
             kpar=list(sigma=0.015),C=50,cross=4)
gene
# the kernel function
kernelf(gene)
# the alpha values
alpha(gene)
# the coefficients
coef(gene)
# the fitted values
fitted(gene)
# the cross validation error
cross(gene)
```

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1ssvm

Least Squares Support Vector Machine

# **Description**

The 1ssvm function is an implementation of the Least Squares SVM. 1ssvm includes a reduced version of Least Squares SVM using a decomposition of the kernel matrix which is calculated by the csi function.

# Usage

```
## S4 method for signature 'formula'
lssvm(x, data=NULL, ..., subset, na.action = na.omit, scaled = TRUE)
## S4 method for signature 'vector'
lssvm(x, ...)
## S4 method for signature 'matrix'
lssvm(x, y, scaled = TRUE, kernel = "rbfdot", kpar = "automatic",
      type = NULL, tau = 0.01, reduced = TRUE, tol = 0.0001,
     rank = floor(dim(x)[1]/3), delta = 40, cross = 0, fit = TRUE,
      ..., subset, na.action = na.omit)
## S4 method for signature 'kernelMatrix'
lssvm(x, y, type = NULL, tau = 0.01,
      tol = 0.0001, rank = floor(dim(x)[1]/3), delta = 40, cross = 0,
     fit = TRUE, ...)
## S4 method for signature 'list'
lssvm(x, y, scaled = TRUE,
     kernel = "stringdot", kpar = list(length=4, lambda = 0.5),
      type = NULL, tau = 0.01, reduced = TRUE, tol = 0.0001,
     rank = floor(dim(x)[1]/3), delta = 40, cross = 0, fit = TRUE,
      ..., subset)
```

### **Arguments**

data

У

x a symbolic description of the model to be fit, a matrix or vector containing the training data when a formula interface is not used or a kernelMatrix or a list of character vectors.

an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'lssvm' is called from.

a response vector with one label for each row/component of x. Can be either a factor (for classification tasks) or a numeric vector (for classification or regression - currently nor supported -).

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scaled

A logical vector indicating the variables to be scaled. If scaled is of length 1, the value is recycled as many times as needed and all non-binary variables are scaled. Per default, data are scaled internally to zero mean and unit variance. The center and scale values are returned and used for later predictions.

type

Type of problem. Either "classification" or "regression". Depending on whether y is a factor or not, the default setting for type is "classification" or "regression" respectively, but can be overwritten by setting an explicit value. (regression is currently not supported)

kernel

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel "Gaussian"
- polydot Polynomial kernel
- · vanilladot Linear kernel
- tanhdot Hyperbolic tangent kernel
- laplacedot Laplacian kernel
- besseldot Bessel kernel
- anovadot ANOVA RBF kernel
- splinedot Spline kernel
- stringdot String kernel

Setting the kernel parameter to "matrix" treats x as a kernel matrix calling the kernelMatrix interface.

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

by passing the function name as an argument.
the list of hyper-parameters (kernel parameters)

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. For valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".
- length, lambda, normalized for the "stringdot" kernel where length is
  the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be
  normalized.

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

kpar can also be set to the string "automatic" which uses the heuristics in sigest to calculate a good sigma value for the Gaussian RBF or Laplace kernel, from the data. (default = "automatic").

kpar

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the regularization parameter (default 0.01)

reduced if set to FALSE the full linear problem of the lssvm is solved, when TRUE a re-

duced method using csi is used.

rank the maximal rank of the decomposed kernel matrix, see csi

delta number of columns of cholesky performed in advance, see csi (default 40)

tol tolerance of termination criterion for the csi function, lower tolerance leads to

more precise approximation but may increase the training time and the decom-

posed matrix size (default: 0.0001)

fit indicates whether the fitted values should be computed and included in the

model or not (default: 'TRUE')

cross if a integer value k>0 is specified, a k-fold cross validation on the training data

is performed to assess the quality of the model: the Mean Squared Error for

regression

subset An index vector specifying the cases to be used in the training sample. (NOTE:

If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

... additional parameters

### Details

Least Squares Support Vector Machines are reformulation to the standard SVMs that lead to solving linear KKT systems. The algorithm is based on the minimization of a classical penalized least-squares cost function. The current implementation approximates the kernel matrix by an incomplete Cholesky factorization obtained by the csi function, thus the solution is an approximation to the exact solution of the lssvm optimization problem. The quality of the solution depends on the approximation and can be influenced by the "rank", "delta", and "tol" parameters.

# Value

An S4 object of class "1ssvm" containing the fitted model, Accessor functions can be used to access the slots of the object (see examples) which include:

alpha the parameters of the "lssvm"

coef the model coefficients (identical to alpha)

b the model offset.

xmatrix the training data used by the model

# Author(s)

Alexandros Karatzoglou

<alexandros.karatzoglou@ci.tuwien.ac.at>

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## References

```
J. A. K. Suykens and J. Vandewalle

Least Squares Support Vector Machine Classifiers

Neural Processing Letters vol. 9, issue 3, June 1999
```

### See Also

```
ksvm, gausspr, csi
```

# **Examples**

```
## simple example
data(iris)
lir <- lssvm(Species~.,data=iris)
lir
lirr <- lssvm(Species~.,data= iris, reduced = FALSE)
lirr

## Using the kernelMatrix interface
iris <- unique(iris)
rbf <- rbfdot(0.5)
k <- kernelMatrix(rbf, as.matrix(iris[,-5]))
klir <- lssvm(k, iris[, 5])
klir
pre <- predict(klir, k)</pre>
```

lssvm-class

Class "lssvm"

# **Description**

The Gaussian Processes object

# **Objects from the Class**

Objects can be created by calls of the form new("lssvm", ...). or by calling the lssvm function

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### **Slots**

```
kernelf: Object of class "kfunction" contains the kernel function used
kpar: Object of class "list" contains the kernel parameter used
param: Object of class "list" contains the regularization parameter used.
kcall: Object of class "call" contains the used function call
type: Object of class "character" contains type of problem
coef: Object of class "ANY" contains the model parameter
terms: Object of class "ANY" contains the terms representation of the symbolic model used (when
     using a formula)
xmatrix: Object of class "matrix" containing the data matrix used
ymatrix: Object of class "output" containing the response matrix
fitted: Object of class "output" containing the fitted values
b: Object of class "numeric" containing the offset
lev: Object of class "vector" containing the levels of the response (in case of classification)
scaling: Object of class "ANY" containing the scaling information performed on the data
nclass: Object of class "numeric" containing the number of classes (in case of classification)
alpha: Object of class "listI" containing the computes alpha values
alphaindex Object of class "list" containing the indexes for the alphas in various classes (in
     multi-class problems).
error: Object of class "numeric" containing the training error
cross: Object of class "numeric" containing the cross validation error
n.action: Object of class "ANY" containing the action performed in NA
nSV: Object of class "numeric" containing the number of model parameters
```

#### Methods

```
alpha signature(object = "lssvm"): returns the alpha vector
cross signature(object = "lssvm"): returns the cross validation error
error signature(object = "lssvm"): returns the training error
fitted signature(object = "vm"): returns the fitted values
kcall signature(object = "lssvm"): returns the call performed
kernelf signature(object = "lssvm"): returns the kernel function used
kpar signature(object = "lssvm"): returns the kernel parameter used
param signature(object = "lssvm"): returns the regularization parameter used
lev signature(object = "lssvm"): returns the response levels (in classification)
type signature(object = "lssvm"): returns the scaling values
xmatrix signature(object = "lssvm"): returns the data matrix used
ymatrix signature(object = "lssvm"): returns the response matrix used
```

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## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
lssvm, ksvm-class
```

## **Examples**

```
# train model
data(iris)
test <- lssvm(Species~.,data=iris,var=2)
test
alpha(test)
error(test)
lev(test)</pre>
```

musk

Musk data set

# Description

This dataset describes a set of 92 molecules of which 47 are judged by human experts to be musks and the remaining 45 molecules are judged to be non-musks.

### Usage

```
data(musk)
```

# **Format**

A data frame with 476 observations on the following 167 variables.

Variables 1-162 are "distance features" along rays. The distances are measured in hundredths of Angstroms. The distances may be negative or positive, since they are actually measured relative to an origin placed along each ray. The origin was defined by a "consensus musk" surface that is no longer used. Hence, any experiments with the data should treat these feature values as lying on an arbitrary continuous scale. In particular, the algorithm should not make any use of the zero point or the sign of each feature value.

Variable 163 is the distance of the oxygen atom in the molecule to a designated point in 3-space. This is also called OXY-DIS.

Variable 164 is the X-displacement from the designated point.

Variable 165 is the Y-displacement from the designated point.

Variable 166 is the Z-displacement from the designated point.

Class: 0 for non-musk, and 1 for musk

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# **Source**

UCI Machine Learning data repository

# **Examples**

```
data(musk)
muskm <- ksvm(Class~.,data=musk,kernel="rbfdot",C=1000)
muskm</pre>
```

onlearn

Kernel Online Learning algorithms

# Description

Online Kernel-based Learning algorithms for classification, novelty detection, and regression.

# Usage

```
## S4 method for signature 'onlearn'
onlearn(obj, x, y = NULL, nu = 0.2, lambda = 1e-04)
```

# **Arguments**

obj	obj an object of class onlearn created by the initialization function inlearn containing the kernel to be used during learning and the parameters of the learned model
X	vector or matrix containing the data. Factors have to be numerically coded. If x is a matrix the code is run internally one sample at the time.
У	the class label in case of classification. Only binary classification is supported and class labels have to be -1 or $\pm 1$ .
nu	the parameter similarly to the nu parameter in SVM bounds the training error.
lambda	the learning rate

# **Details**

The online algorithms are based on a simple stochastic gradient descent method in feature space. The state of the algorithm is stored in an object of class onlearn and has to be passed to the function at each iteration.

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## Value

The function returns an S4 object of class onlearn containing the model parameters and the last fitted value which can be retrieved by the accessor method fit. The value returned in the classification and novelty detection problem is the decision function value phi. The accessor methods alpha returns the model parameters.

# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

## References

```
Kivinen J. Smola A.J. Williamson R.C. Online Learning with Kernels
IEEE Transactions on Signal Processing vol. 52, Issue 8, 2004 https://alex.smola.org/papers/2004/KivSmoWil04.pdf
```

### See Also

inlearn

## **Examples**

onlearn-class

Class "onlearn"

## **Description**

The class of objects used by the Kernel-based Online learning algorithms

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## **Objects from the Class**

Objects can be created by calls of the form new("onlearn", ...). or by calls to the function inlearn.

#### Slots

```
kernelf: Object of class "function" containing the used kernel function
buffer: Object of class "numeric" containing the size of the buffer
kpar: Object of class "list" containing the hyperparameters of the kernel function.
xmatrix: Object of class "matrix" containing the data points (similar to support vectors)
fit: Object of class "numeric" containing the decision function value of the last data point
onstart: Object of class "numeric" used for indexing
onstop: Object of class "numeric" used for indexing
alpha: Object of class "ANY" containing the model parameters
rho: Object of class "numeric" containing model parameter
b: Object of class "numeric" containing the offset
pattern: Object of class "factor" used for dealing with factors
type: Object of class "character" containing the problem type (classification, regression, or novelty
```

#### Methods

```
alpha signature(object = "onlearn"): returns the model parameters
b signature(object = "onlearn"): returns the offset
buffer signature(object = "onlearn"): returns the buffer size
fit signature(object = "onlearn"): returns the last decision function value
kernelf signature(object = "onlearn"): return the kernel function used
kpar signature(object = "onlearn"): returns the hyper-parameters used
onlearn signature(obj = "onlearn"): the learning function
predict signature(object = "onlearn"): the predict function
rho signature(object = "onlearn"): returns model parameter
show signature(object = "onlearn"): show function
type signature(object = "onlearn"): returns the type of problem
xmatrix signature(object = "onlearn"): returns the stored data points
```

### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

## See Also

```
onlearn, inlearn
```

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# **Examples**

plot

plot method for support vector object

# **Description**

Plot a binary classification support vector machine object. The plot function returns a contour plot of the decision values.

# Usage

```
## S4 method for signature 'ksvm'
plot(object, data=NULL, grid = 50, slice = list())
```

## **Arguments**

object a ksvm classification object created by the ksvm function
data a data frame or matrix containing data to be plotted
grid granularity for the contour plot.
slice a list of named numeric values for the dimensions held constant (only needed if more than two variables are used). Dimensions not specified are fixed at 0.

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

### See Also

ksvm

prc-class 73

# **Examples**

```
## Demo of the plot function
x <- rbind(matrix(rnorm(120),,2),matrix(rnorm(120,mean=3),,2))
y <- matrix(c(rep(1,60),rep(-1,60)))

svp <- ksvm(x,y,type="C-svc")
plot(svp,data=x)</pre>
```

prc-class

Class "prc"

# **Description**

Principal Components Class

# Objects of class "prc"

Objects from the class cannot be created directly but only contained in other classes.

#### **Slots**

```
pcv: Object of class "matrix" containing the principal component vectors eig: Object of class "vector" containing the corresponding eigenvalues kernelf: Object of class "kfunction" containing the kernel function used kpar: Object of class "list" containing the kernel parameters used xmatrix: Object of class "input" containing the data matrix used kcall: Object of class "ANY" containing the function call n.action: Object of class "ANY" containing the action performed on NA
```

# Methods

```
eig signature(object = "prc"): returns the eigenvalues
kcall signature(object = "prc"): returns the performed call
kernelf signature(object = "prc"): returns the used kernel function
pcv signature(object = "prc"): returns the principal component vectors
predict signature(object = "prc"): embeds new data
xmatrix signature(object = "prc"): returns the used data matrix
```

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
kpca-class,kha-class,kfa-class
```

74 predict.gausspr

Gaussian Processes object

predict.gausspr	predict method for
p. carco. Saacop.	product memory or

# Description

Prediction of test data using Gaussian Processes

#### Usage

```
## S4 method for signature 'gausspr'
predict(object, newdata, type = "response", coupler = "minpair")
```

# **Arguments**

object an S4 object of class gausspr created by the gausspr function

newdata a data frame or matrix containing new data

type one of response, probabilities indicating the type of output: predicted val-

ues or matrix of class probabilities

coupler Coupling method used in the multiclass case, can be one of minpair or pkpd

(see reference for more details).

# Value

response predicted classes (the classes with majority vote) or the response value in regres-

sion.

probabilities matrix of class probabilities (one column for each class and one row for each

input).

# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### References

C. K. I. Williams and D. Barber
Bayesian classification with Gaussian processes.
IEEE Transactions on Pattern Analysis and Machine Intelligence, 20(12):1342-1351, 1998
<a href="https://homepages.inf.ed.ac.uk/ckiw/postscript/pami\_final.ps.gz">https://homepages.inf.ed.ac.uk/ckiw/postscript/pami\_final.ps.gz</a>

• T.F. Wu, C.J. Lin, R.C. Weng.

Probability estimates for Multi-class Classification by Pairwise Coupling

https://www.csie.ntu.edu.tw/~cjlin/papers/svmprob/svmprob.pdf

predict.kqr 75

# **Examples**

predict.kgr

Predict method for kernel Quantile Regression object

# **Description**

Prediction of test data for kernel quantile regression

# Usage

```
## S4 method for signature 'kqr'
predict(object, newdata)
```

# Arguments

object an S4 object of class kqr created by the kqr function newdata a data frame, matrix, or kernelMatrix containing new data

## Value

The value of the quantile given by the computed kqr model in a vector of length equal to the the rows of newdata.

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

76 predict.ksvm

#### **Examples**

predict.ksvm

predict method for support vector object

# **Description**

Prediction of test data using support vector machines

# Usage

```
## S4 method for signature 'ksvm'
predict(object, newdata, type = "response", coupler = "minpair")
```

# **Arguments**

object an S4 object of class ksvm created by the ksvm function

newdata a data frame or matrix containing new data

type one of response, probabilities, votes, decision indicating the type of out-

put: predicted values, matrix of class probabilities, matrix of vote counts, or

matrix of decision values.

coupler Coupling method used in the multiclass case, can be one of minpair or pkpd

(see reference for more details).

# Value

If type(object) is C-svc, nu-svc, C-bsvm or spoc-svc the vector returned depends on the argument type:

response predicted classes (the classes with majority vote).

promotergene 77

probabilities matrix of class probabilities (one column for each class and one row for each input).

votes matrix of vote counts (one column for each class and one row for each new input)

If type(object) is eps-svr, eps-bsvr or nu-svr a vector of predicted values is returned. If type(object) is one-classification a vector of logical values is returned.

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### References

- T.F. Wu, C.J. Lin, R.C. Weng.

  Probability estimates for Multi-class Classification by Pairwise Coupling

  https://www.csie.ntu.edu.tw/~cjlin/papers/svmprob/svmprob.pdf
- H.T. Lin, C.J. Lin, R.C. Weng (2007), A note on Platt's probabilistic outputs for support vector machines. *Machine Learning*, **68**, 267–276. doi:10.1007/s1099400750186.

# **Examples**

promotergene

E. coli promoter gene sequences (DNA)

# **Description**

Promoters have a region where a protein (RNA polymerase) must make contact and the helical DNA sequence must have a valid conformation so that the two pieces of the contact region spatially align. The data contains DNA sequences of promoters and non-promoters.

78 ranking

#### Usage

```
data(promotergene)
```

#### **Format**

A data frame with 106 observations and 58 variables. The first variable Class is a factor with levels + for a promoter gene and - for a non-promoter gene. The remaining 57 variables V2 to V58 are factors describing the sequence. The DNA bases are coded as follows: a adenine c cytosine g guanine t thymine

#### **Source**

doi:10.24432/C5S01D

#### References

Towell, G., Shavlik, J. and Noordewier, M. Refinement of Approximate Domain Theories by Knowledge-Based Artificial Neural Networks. In Proceedings of the Eighth National Conference on Artificial Intelligence (AAAI-90)

# **Examples**

ranking

Ranking

# **Description**

A universal ranking algorithm which assigns importance/ranking to data points given a query.

ranking 79

#### **Usage**

# **Arguments**

x a matrix containing the data to be ranked, or the kernel matrix of data to be ranked or a list of character vectors

The index of the query point in the data matrix or a vector of length equal to the rows of the data matrix having a one at the index of the query points index and zero at all the other points.

the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- anovadot ANOVA RBF kernel function
- splinedot Spline kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. For valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"

v

У

kernel

kpar

80 ranking

• sigma, order, degree for the Bessel kernel "besseldot".

• sigma, degree for the ANOVA kernel "anovadot".

Hyper-parameters for user defined kernels can be passed through the kpar pa-

rameter as well.

scale If TRUE the data matrix columns are scaled to zero mean and unit variance.

alpha The alpha parameter takes values between 0 and 1 and is used to control the

authoritative scores received from the unlabeled points. For 0 no global structure is found the algorithm ranks the points similarly to the original distance metric.

iterations Maximum number of iterations

edgegraph Construct edgegraph (only supported with the RBF kernel)

convergence Include convergence matrix in results

. . . Additional arguments

#### **Details**

A simple universal ranking algorithm which exploits the intrinsic global geometric structure of the data. In many real world applications this should be superior to a local method in which the data are simply ranked by pairwise Euclidean distances. Firstly a weighted network is defined on the data and an authoritative score is assigned to each query. The query points act as source nodes that continually pump their authoritative scores to the remaining points via the weighted network and the remaining points further spread the scores they received to their neighbors. This spreading process is repeated until convergence and the points are ranked according to their score at the end of the iterations.

# Value

An S4 object of class ranking which extends the matrix class. The first column of the returned matrix contains the original index of the points in the data matrix the second column contains the final score received by each point and the third column the ranking of the point. The object contains the following slots:

edgegraph Containing the edgegraph of the data points.

convergence Containing the convergence matrix

#### Author(s)

Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>

#### References

D. Zhou, J. Weston, A. Gretton, O. Bousquet, B. Schoelkopf *Ranking on Data Manifolds*Advances in Neural Information Processing Systems 16.
MIT Press Cambridge Mass. 2004

https://papers.neurips.cc/paper/2447-ranking-on-data-manifolds.pdf

ranking-class 81

#### See Also

```
ranking-class, specc
```

## **Examples**

ranking-class

Class "ranking"

# Description

Object of the class "ranking" are created from the ranking function and extend the class matrix

#### **Objects from the Class**

Objects can be created by calls of the form new("ranking", ...).

# **Slots**

```
.Data: Object of class "matrix" containing the data ranking and scores convergence: Object of class "matrix" containing the convergence matrix edgegraph: Object of class "matrix" containing the edgegraph
```

# Extends

```
Class "matrix", directly.
```

#### Methods

```
show signature(object = "ranking"): displays the ranking score matrix
```

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

82 reuters

# See Also

```
ranking
```

# **Examples**

reuters

Reuters Text Data

# Description

A small sample from the Reuters news data set.

#### Usage

```
data(reuters)
```

# **Format**

A list of 40 text documents along with the labels. reuters contains the text documents and rlabels the labels in a vector.

## **Details**

This dataset contains a list of 40 text documents along with the labels. The data consist out of 20 documents from the acq category and 20 documents from the crude category. The labels are stored in rlabels

#### Source

Reuters

83 rvm

rvm

Relevance Vector Machine

# **Description**

The Relevance Vector Machine is a Bayesian model for regression and classification of identical functional form to the support vector machine. The rvm function currently supports only regression.

# Usage

```
## S4 method for signature 'formula'
rvm(x, data=NULL, ..., subset, na.action = na.omit)
## S4 method for signature 'vector'
rvm(x, ...)
## S4 method for signature 'matrix'
rvm(x, y, type="regression",
   kernel="rbfdot", kpar="automatic",
   alpha= ncol(as.matrix(x)), var=0.1, var.fix=FALSE, iterations=100,
   verbosity = 0, tol = .Machine$double.eps, minmaxdiff = 1e-3,
   cross = 0, fit = TRUE, ..., subset, na.action = na.omit)
## S4 method for signature 'list'
rvm(x, y, type = "regression",
   kernel = "stringdot", kpar = list(length = 4, lambda = 0.5),
   alpha = 5, var = 0.1, var.fix = FALSE, iterations = 100,
   verbosity = 0, tol = .Machine$double.eps, minmaxdiff = 1e-3,
   cross = 0, fit = TRUE, ..., subset, na.action = na.omit)
```

# **Arguments**

У

kernel

x	a symbolic description of the model to be fit. When not using a formula x can
	be a matrix or vector containing the training data or a kernel matrix of class
	kernelMatrix of the training data or a list of character vectors (for use with the
	string kernel). Note, that the intercept is always excluded, whether given in the
	formula or not.
data	an optional data frame containing the variables in the model. By default the

variables are taken from the environment which 'rvm' is called from.

a response vector with one label for each row/component of x. Can be either a factor (for classification tasks) or a numeric vector (for regression).

type rvm can only be used for regression at the moment.

> the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

84 rvm

- rbfdot Radial Basis kernel "Gaussian"
- polydot Polynomial kernel
- · vanilladot Linear kernel
- tanhdot Hyperbolic tangent kernel
- laplacedot Laplacian kernel
- besseldot Bessel kernel
- · anovadot ANOVA RBF kernel
- splinedot Spline kernel
- stringdot String kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. For valid parameters for existing kernels are :

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".
- length, lambda, normalized for the "stringdot" kernel where length is
  the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be
  normalized.

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well. In the case of a Radial Basis kernel function (Gaussian) kpar can also be set to the string "automatic" which uses the heuristics in sigest to calculate a good sigma value for the Gaussian RBF or Laplace kernel, from the data. (default = "automatic").

alpha

The initial alpha vector. Can be either a vector of length equal to the number of data points or a single number.

var

the initial noise variance

var.fix

Keep noise variance fix during iterations (default: FALSE)

iterations

Number of iterations allowed (default: 100)

tol

tolerance of termination criterion

minmaxdiff

termination criteria. Stop when max difference is equal to this parameter (default:1e-3)

verbosity

print information on algorithm convergence (default = FALSE)

fit

indicates whether the fitted values should be computed and included in the model or not (default: TRUE)

cross

if a integer value k>0 is specified, a k-fold cross validation on the training data is performed to assess the quality of the model: the Mean Squared Error for regression

rvm 85

subset An index vector specifying the cases to be used in the training sample. (NOTE:

If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default action is

na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found.

(NOTE: If given, this argument must be named.)

... additional parameters

#### **Details**

The Relevance Vector Machine typically leads to sparser models then the SVM. It also performs better in many cases (specially in regression).

#### Value

An S4 object of class "rvm" containing the fitted model. Accessor functions can be used to access the slots of the object which include :

alpha The resulting relevance vectors

alphaindex The index of the resulting relevance vectors in the data matrix

nRV Number of relevance vectors

RVindex The indexes of the relevance vectors

error Training error (if fit = TRUE)

...

## Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### References

```
Tipping, M. E.
```

Sparse Bayesian learning and the relevance vector machine

Journal of Machine Learning Research 1, 211-244

https://www.jmlr.org/papers/volume1/tipping01a/tipping01a.pdf

#### See Also

ksvm

# **Examples**

```
# create data
x <- seq(-20,20,0.1)
y <- sin(x)/x + rnorm(401,sd=0.05)
# train relevance vector machine</pre>
```

86 rvm-class

```
foo <- rvm(x, y)
foo
# print relevance vectors
alpha(foo)
RVindex(foo)

# predict and plot
ytest <- predict(foo, x)
plot(x, y, type ="1")
lines(x, ytest, col="red")</pre>
```

rvm-class

Class "rvm"

#### **Description**

Relevance Vector Machine Class

## **Objects from the Class**

Objects can be created by calls of the form new("rvm", ...). or by calling the rvm function.

#### **Slots**

tol: Object of class "numeric" contains tolerance of termination criteria used. kernelf: Object of class "kfunction" contains the kernel function used kpar: Object of class "list" contains the hyperparameter used kcall: Object of class "call" contains the function call type: Object of class "character" contains type of problem terms: Object of class "ANY" containing the terms representation of the symbolic model used (when using a formula interface) xmatrix: Object of class "matrix" contains the data matrix used during computation ymatrix: Object of class "output" contains the response matrix fitted: Object of class "output" with the fitted values, (predict on training set). lev: Object of class "vector" contains the levels of the response (in classification) nclass: Object of class "numeric" contains the number of classes (in classification) alpha: Object of class "listI" containing the the resulting alpha vector coef: Object of class "ANY" containing the the resulting model parameters nvar: Object of class "numeric" containing the calculated variance (in case of regression) mlike: Object of class "numeric" containing the computed maximum likelihood RVindex: Object of class "vector" containing the indexes of the resulting relevance vectors nRV: Object of class "numeric" containing the number of relevance vectors cross: Object of class "numeric" containing the resulting cross validation error error: Object of class "numeric" containing the training error

n.action: Object of class "ANY" containing the action performed on NA

rvm-class 87

#### Methods

```
RVindex signature(object = "rvm"): returns the index of the relevance vectors
alpha signature(object = "rvm"): returns the resulting alpha vector
cross signature(object = "rvm"): returns the resulting cross validation error
error signature(object = "rvm"): returns the training error
fitted signature(object = "rvm"): returns the fitted values
kcall signature(object = "rvm"): returns the function call
kernelf signature(object = "rvm"): returns the used kernel function
kpar signature(object = "rvm"): returns the parameters of the kernel function
lev signature(object = "rvm"): returns the levels of the response (in classification)
mlike signature(object = "rvm"): returns the estimated maximum likelihood
nvar signature(object = "rvm"): returns the calculated variance (in regression)
type signature(object = "rvm"): returns the type of problem
xmatrix signature(object = "rvm"): returns the data matrix used during computation
ymatrix signature(object = "rvm"): returns the used response
```

# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

## See Also

```
rvm, ksvm-class
```

#### **Examples**

```
# create data
x <- seq(-20,20,0.1)
y <- sin(x)/x + rnorm(401,sd=0.05)
# train relevance vector machine
foo <- rvm(x, y)
foo
alpha(foo)
RVindex(foo)
fitted(foo)
kernelf(foo)
nvar(foo)
## show slots
slotNames(foo)</pre>
```

88 sigest

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31	50	0	ι

Hyperparameter estimation for the Gaussian Radial Basis kernel

# Description

Given a range of values for the "sigma" inverse width parameter in the Gaussian Radial Basis kernel for use with Support Vector Machines. The estimation is based on the data to be used.

# Usage

```
## S4 method for signature 'formula'
sigest(x, data=NULL, frac = 0.5, na.action = na.omit, scaled = TRUE)
## S4 method for signature 'matrix'
sigest(x, frac = 0.5, scaled = TRUE, na.action = na.omit)
```

# **Arguments**

x	a symbolic description of the model upon the estimation is based. When not using a formula x is a matrix or vector containing the data
data	an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'ksvm' is called from.
frac	Fraction of data to use for estimation. By default a quarter of the data is used to estimate the range of the sigma hyperparameter.
scaled	A logical vector indicating the variables to be scaled. If scaled is of length 1, the value is recycled as many times as needed and all non-binary variables are scaled. Per default, data are scaled internally to zero mean and unit variance (since this the default action in ksvm as well). The center and scale values are returned and used for later predictions.
na.action	A function to specify the action to be taken if NAs are found. The default action is na.omit, which leads to rejection of cases with missing values on any required variable. An alternative is na.fail, which causes an error if NA cases are found. (NOTE: If given, this argument must be named.)

#### **Details**

sigest estimates the range of values for the sigma parameter which would return good results when used with a Support Vector Machine (ksvm). The estimation is based upon the 0.1 and 0.9 quantile of  $||x - x'||^2$ . Basically any value in between those two bounds will produce good results.

#### Value

Returns a vector of length 3 defining the range (0.1 quantile, median and 0.9 quantile) of the sigma hyperparameter.

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#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### References

B. Caputo, K. Sim, F. Furesjo, A. Smola,

Appearance-based object recognition using SVMs: which kernel should I use?

Proc of NIPS workshop on Statistical methods for computational experiments in visual processing and computer vision, Whistler, 2002.

#### See Also

ksvm

#### **Examples**

```
## estimate good sigma values for promotergene
data(promotergene)
srange <- sigest(Class~.,data = promotergene)</pre>
srange
s <- srange[2]
## create test and training set
ind <- sample(1:dim(promotergene)[1],20)</pre>
genetrain <- promotergene[-ind, ]</pre>
genetest <- promotergene[ind, ]</pre>
## train a support vector machine
gene <- ksvm(Class~.,data=genetrain,kernel="rbfdot",</pre>
              kpar=list(sigma = s),C=50,cross=3)
gene
## predict gene type on the test set
promoter <- predict(gene,genetest[,-1])</pre>
## Check results
table(promoter,genetest[,1])
```

spam

Spam E-mail Database

# **Description**

A data set collected at Hewlett-Packard Labs, that classifies 4601 e-mails as spam or non-spam. In addition to this class label there are 57 variables indicating the frequency of certain words and characters in the e-mail.

90 specc

#### Usage

data(spam)

#### **Format**

A data frame with 4601 observations and 58 variables.

The first 48 variables contain the frequency of the variable name (e.g., business) in the e-mail. If the variable name starts with num (e.g., num650) the it indicates the frequency of the corresponding number (e.g., 650). The variables 49-54 indicate the frequency of the characters ';', '(', '[', '!', 's', and '#'. The variables 55-57 contain the average, longest and total run-length of capital letters. Variable 58 indicates the type of the mail and is either "nonspam" or "spam", i.e. unsolicited commercial e-mail.

#### **Details**

The data set contains 2788 e-mails classified as "nonspam" and 1813 classified as "spam".

The "spam" concept is diverse: advertisements for products/web sites, make money fast schemes, chain letters, pornography... This collection of spam e-mails came from the collectors' postmaster and individuals who had filed spam. The collection of non-spam e-mails came from filed work and personal e-mails, and hence the word 'george' and the area code '650' are indicators of non-spam. These are useful when constructing a personalized spam filter. One would either have to blind such non-spam indicators or get a very wide collection of non-spam to generate a general purpose spam filter.

#### Source

doi:10.24432/C53G6X

#### References

T. Hastie, R. Tibshirani, J.H. Friedman. The Elements of Statistical Learning. Springer, 2001.

specc

Spectral Clustering

## **Description**

A spectral clustering algorithm. Clustering is performed by embedding the data into the subspace of the eigenvectors of an affinity matrix.

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#### **Usage**

#### **Arguments**

Х

the matrix of data to be clustered, or a symbolic description of the model to be fit, or a kernel Matrix of class kernelMatrix, or a list of character vectors.

data

an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'specc' is called from.

centers

Either the number of clusters or a set of initial cluster centers. If the first, a random set of rows in the eigenvectors matrix are chosen as the initial centers.

kernel

the kernel function used in computing the affinity matrix. This parameter can be set to any function, of class kernel, which computes a dot product between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfdot Radial Basis kernel function "Gaussian"
- polydot Polynomial kernel function
- vanilladot Linear kernel function
- tanhdot Hyperbolic tangent kernel function
- laplacedot Laplacian kernel function
- besseldot Bessel kernel function
- · anovadot ANOVA RBF kernel function
- splinedot Spline kernel
- stringdot String kernel

The kernel parameter can also be set to a user defined function of class kernel by passing the function name as an argument.

kpar

a character string or the list of hyper-parameters (kernel parameters). The default character string "automatic" uses a heuristic to determine a suitable value for the width parameter of the RBF kernel. The second option "local" (local

92 specc

scaling) uses a more advanced heuristic and sets a width parameter for every point in the data set. This is particularly useful when the data incorporates multiple scales. A list can also be used containing the parameters to be used with the kernel function. Valid parameters for existing kernels are:

- sigma inverse kernel width for the Radial Basis kernel function "rbfdot" and the Laplacian kernel "laplacedot".
- degree, scale, offset for the Polynomial kernel "polydot"
- scale, offset for the Hyperbolic tangent kernel function "tanhdot"
- sigma, order, degree for the Bessel kernel "besseldot".
- sigma, degree for the ANOVA kernel "anovadot".
- length, lambda, normalized for the "stringdot" kernel where length is
  the length of the strings considered, lambda the decay factor and normalized a logical parameter determining if the kernel evaluations should be
  normalized.

Hyper-parameters for user defined kernels can be passed through the kpar parameter as well.

nystrom.red

use nystrom method to calculate eigenvectors. When TRUE a sample of the dataset is used to calculate the eigenvalues, thus only a nxm matrix where n the sample size is stored in memory (default: FALSE

nystrom.sample

number of data points to use for estimating the eigenvalues when using the nys-

trom method. (default : dim(x)[1]/6)

mod.sample proportion of data to use when estimating sigma (default: 0.75)

iterations the maximum number of iterations allowed.

na.action the action to perform on NA

... additional parameters

#### Details

Spectral clustering works by embedding the data points of the partitioning problem into the subspace of the k largest eigenvectors of a normalized affinity/kernel matrix. Using a simple clustering method like kmeans on the embedded points usually leads to good performance. It can be shown that spectral clustering methods boil down to graph partitioning.

The data can be passed to the specc function in a matrix or a data.frame, in addition specc also supports input in the form of a kernel matrix of class kernelMatrix or as a list of character vectors where a string kernel has to be used.

#### Value

An S4 object of class specc which extends the class vector containing integers indicating the cluster to which each point is allocated. The following slots contain useful information

centers A matrix of cluster centers.

size The number of point in each cluster

withinss The within-cluster sum of squares for each cluster

kernelf The kernel function used

specc-class 93

#### Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### References

```
Andrew Y. Ng, Michael I. Jordan, Yair Weiss

On Spectral Clustering: Analysis and an Algorithm

Neural Information Processing Symposium 2001

https://papers.neurips.cc/paper/2092-on-spectral-clustering-analysis-and-an-algorithm.

pdf
```

#### See Also

kkmeans, kpca, kcca

## **Examples**

```
## Cluster the spirals data set.
data(spirals)

sc <- specc(spirals, centers=2)

sc 
centers(sc)
size(sc)
withinss(sc)

plot(spirals, col=sc)</pre>
```

specc-class

Class "specc"

# **Description**

The Spectral Clustering Class

## **Objects from the Class**

Objects can be created by calls of the form new("specc", ...). or by calling the function specc.

#### **Slots**

```
.Data: Object of class "vector" containing the cluster assignments centers: Object of class "matrix" containing the cluster centers size: Object of class "vector" containing the number of points in each cluster withinss: Object of class "vector" containing the within-cluster sum of squares for each cluster kernelf Object of class kernel containing the used kernel function.
```

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#### Methods

```
centers signature(object = "specc"): returns the cluster centers
withinss signature(object = "specc"): returns the within-cluster sum of squares for each cluster
ter
size signature(object = "specc"): returns the number of points in each cluster
```

# Author(s)

```
Alexandros Karatzoglou <alexandros.karatzoglou@ci.tuwien.ac.at>
```

#### See Also

```
specc, kpca-class
```

# **Examples**

```
## Cluster the spirals data set.
data(spirals)
sc <- specc(spirals, centers=2)
centers(sc)
size(sc)</pre>
```

spirals

Spirals Dataset

# Description

A toy data set representing two spirals with Gaussian noise. The data was created with the mlbench. spirals function in mlbench.

# Usage

```
data(spirals)
```

## **Format**

A matrix with 300 observations and 2 variables.

# **Examples**

```
data(spirals)
plot(spirals)
```

stringdot 95

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String Kernel Functions

# Description

String kernels.

#### Usage

```
stringdot(length = 4, lambda = 1.1, type = "spectrum", normalized = TRUE)
```

# **Arguments**

length The length of the substrings considered

lambda The decay factor

type Type of string kernel, currently the following kernels are supported:

spectrum the kernel considers only matching substring of exactly length n (also know as string kernel). Each such matching substring is given a constant weight. The length parameter in this kernel has to be length > 1.

boundrange this kernel (also known as boundrange) considers only matching substrings of length less than or equal to a given number N. This type of string kernel requires a length parameter length>1

constant The kernel considers all matching substrings and assigns constant weight (e.g. 1) to each of them. This constant kernel does not require any additional parameter.

exponential Exponential Decay kernel where the substring weight decays as the matching substring gets longer. The kernel requires a decay factor  $\lambda>1$ 

string essentially identical to the spectrum kernel, only computed using a more conventional way.

fullstring essentially identical to the boundrange kernel only computed in a more conventional way.

normalized

normalize string kernel values, (default: TRUE)

#### **Details**

The kernel generating functions are used to initialize a kernel function which calculates the dot (inner) product between two feature vectors in a Hilbert Space. These functions or their function generating names can be passed as a kernel argument on almost all functions in **kernlab**(e.g., ksvm, kpca etc.).

96 ticdata

The string kernels calculate similarities between two strings (e.g. texts or sequences) by matching the common substring in the strings. Different types of string kernel exists and are mainly distinguished by how the matching is performed i.e. some string kernels count the exact matchings of n characters (spectrum kernel) between the strings, others allow gaps (mismatch kernel) etc.

#### Value

Returns an S4 object of class stringkernel which extents the function class. The resulting function implements the given kernel calculating the inner (dot) product between two character vectors.

kpar a list containing the kernel parameters (hyperparameters) used.

The kernel parameters can be accessed by the kpar function.

#### Note

The spectrum and boundrange kernel are faster and more efficient implementations of the string and fullstring kernels which will be still included in kernlab for the next two versions.

#### Author(s)

```
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```

#### See Also

```
dots, kernelMatrix, kernelMult, kernelPol
```

# **Examples**

```
sk <- stringdot(type="string", length=5)
sk</pre>
```

ticdata

The Insurance Company Data

# **Description**

This data set used in the CoIL 2000 Challenge contains information on customers of an insurance company. The data consists of 86 variables and includes product usage data and socio-demographic data derived from zip area codes. The data was collected to answer the following question: Can you predict who would be interested in buying a caravan insurance policy and give an explanation why

ticdata 97

# Usage

data(ticdata)

#### **Format**

ticdata: Dataset to train and validate prediction models and build a description (9822 customer records). Each record consists of 86 attributes, containing sociodemographic data (attribute 1-43) and product ownership (attributes 44-86). The sociodemographic data is derived from zip codes. All customers living in areas with the same zip code have the same sociodemographic attributes. Attribute 86, CARAVAN: Number of mobile home policies, is the target variable.

#### Data Format

1	STYPE	Customer Subture
2	MAANTHUI	Customer Subtype Number of houses 1 - 10
3	MGEMOMV	
<i>3</i>		Avg size household 1 - 6
5	MGEMLEEF	Average age
	MOSHOOFD	Customer main type
6	MGODRK	Roman catholic
7	MGODPR	Protestant
8	MGODOV	Other religion
9	MGODGE	No religion
10	MRELGE	Married
11	MRELSA	Living together
12	MRELOV	Other relation
13		Singles
14	MFGEKIND	Household without children
15	MFWEKIND	Household with children
16	MOPLH00G	High level education
17	MOPLMIDD	Medium level education
18	MOPLLAAG	Lower level education
19	MBERH00G	High status
20	MBERZELF	Entrepreneur
21	MBERB0ER	Farmer
22	MBERMIDD	Middle management
23	MBERARBG	Skilled labourers
24	MBERARBO	Unskilled labourers
25	MSKA	Social class A
26	MSKB1	Social class B1
27	MSKB2	Social class B2
28	MSKC	Social class C
29	MSKD	Social class D
30	MHHUUR	Rented house
31	MHKOOP	Home owners
32	MAUT1	1 car
33	MAUT2	2 cars
34	MAUT0	No car
35	MZFONDS	National Health Service
36	MZPART	Private health insurance
50	1141 /1111	i ii vate ileatui ilisurailee

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37	MINKM30	Income >30.000
38	MINK3045	Income 30-45,000
39	MINK4575	Income 45-75.000
40	MINK7512	Income 75-122.000
41	MINK123M	Income <123.000
42	MINKGEM	Average income
43	MKOOPKLA	Purchasing power class
44	PWAPART	Contribution private third party insurance
45	PWABEDR	Contribution third party insurance (firms)
46	PWALAND	Contribution third party insurance (agriculture)
47	PPERSAUT	Contribution car policies
48	PBESAUT	Contribution delivery van policies
49	PMOTSCO	Contribution motorcycle/scooter policies
50	PVRAAUT	Contribution lorry policies
51	PAANHANG	Contribution trailer policies
52	PTRACTOR	Contribution tractor policies
53	PWERKT	Contribution agricultural machines policies
54	PBROM	Contribution moped policies
55	PLEVEN	Contribution life insurances
56	PPERSONG	Contribution private accident insurance policies
57	PGEZONG	Contribution family accidents insurance policies
58	PWAOREG	Contribution disability insurance policies
59	PBRAND	Contribution fire policies
60	PZEILPL	Contribution surfboard policies
61	PPLEZIER	Contribution boat policies
62	PFIETS	Contribution bicycle policies
63	PINBOED	Contribution property insurance policies
64	PBYSTAND	Contribution social security insurance policies
65	AWAPART	Number of private third party insurance 1 - 12
	AWABEDR	Number of third party insurance (firms)
	AWALAND	Number of third party insurance (agriculture)
	APERSAUT	Number of car policies
69	ABESAUT	Number of delivery van policies
	AMOTSCO	Number of motorcycle/scooter policies
	AVRAAUT	Number of lorry policies
	AAANHANG	Number of trailer policies
73	ATRACTOR	Number of tractor policies
74	AWERKT	Number of agricultural machines policies
75	ABROM	Number of moped policies
76	ALEVEN	Number of life insurances
77	APERSONG	Number of private accident insurance policies
78	AGEZONG	Number of family accidents insurance policies
79	AWAOREG	Number of disability insurance policies
80	ABRAND	Number of fire policies
81	AZEILPL	Number of surfboard policies
82	APLEZIER	Number of boat policies
83	AFIETS	Number of bicycle policies
84	AINBOED	Number of property insurance policies
		1 1 7 1

vm-class 99

85 ABYSTAND Number of social security insurance policies86 CARAVAN Number of mobile home policies 0 - 1

Note: All the variables starting with M are zipcode variables. They give information on the distribution of that variable, e.g., Rented house, in the zipcode area of the customer.

#### **Details**

Information about the insurance company customers consists of 86 variables and includes product usage data and socio-demographic data derived from zip area codes. The data was supplied by the Dutch data mining company Sentient Machine Research and is based on a real world business problem. The training set contains over 5000 descriptions of customers, including the information of whether or not they have a caravan insurance policy. The test set contains 4000 customers. The test and data set are merged in the ticdata set. More information about the data set and the CoIL 2000 Challenge along with publications based on the data set can be found at http://www.liacs.nl/~putten/library/cc2000/.

#### Source

- UCI KDD Archive:http://kdd.ics.uci.edu
- Donor: Sentient Machine Research
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#### References

Peter van der Putten, Michel de Ruiter, Maarten van Someren Coll Challenge 2000 Tasks and Results: Predicting and Explaining Caravan Policy Ownership http://www.liacs.nl/~putten/library/cc2000/

vm-class Class "vm"

# **Description**

An S4 VIRTUAL class used as a base for the various vector machine classes in **kernlab** 

# **Objects from the Class**

Objects from the class cannot be created directly but only contained in other classes.

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#### **Slots**

```
alpha: Object of class "listI" containing the resulting alpha vector (list in case of multiclass
    classification) (support vectors)
type: Object of class "character" containing the vector machine type e.g., ("C-svc", "nu-svc",
     "C-bsvc", "spoc-svc", "one-svc", "eps-svr", "nu-svr", "eps-bsvr")
kernelf: Object of class "function" containing the kernel function
kpar: Object of class "list" containing the kernel function parameters (hyperparameters)
kcall: Object of class "call" containing the function call
terms: Object of class "ANY" containing the terms representation of the symbolic model used
     (when using a formula)
xmatrix: Object of class "input" the data matrix used during computations (support vectors)
     (possibly scaled and without NA)
ymatrix: Object of class "output" the response matrix/vector
fitted: Object of class "output" with the fitted values, predictions using the training set.
lev: Object of class "vector" with the levels of the response (in the case of classification)
nclass: Object of class "numeric" containing the number of classes (in the case of classification)
error: Object of class "vector" containing the training error
cross: Object of class "vector" containing the cross-validation error
n.action: Object of class "ANY" containing the action performed for NA
```

#### Methods

```
alpha signature(object = "vm"): returns the complete alpha vector (wit zero values)
cross signature(object = "vm"): returns the cross-validation error
error signature(object = "vm"): returns the training error
fitted signature(object = "vm"): returns the fitted values (predict on training set)
kernelf signature(object = "vm"): returns the kernel function
kpar signature(object = "vm"): returns the kernel parameters (hyperparameters)
lev signature(object = "vm"): returns the levels in case of classification
kcall signature(object = "vm"): returns the function call
type signature(object = "vm"): returns the problem type
xmatrix signature(object = "vm"): returns the data matrix used(support vectors)
ymatrix signature(object = "vm"): returns the response vector
```

#### Author(s)

```
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```

#### See Also

```
ksvm-class, rvm-class, gausspr-class
```

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