Package 'kernlab'

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Title Kernel-Based Machine Learning Lab

Description Kernel-based machine learning methods for classification, regression, clustering, novelty detection, quantile regression and dimensionality reduction. Among other methods 'kernlab' includes Support Vector Machines, Spectral Clustering, Kernel PCA, Gaussian Processes and a QP solver.

Depends R (>= 2.10)

Imports methods, stats, grDevices, graphics

LazyLoad Yes

License GPL-2

NeedsCompilation yes

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Contents

kernelMatrix	. 3
uple	
i	. 5
i-class	
ts	
usspr	. 11
usspr-class	
chol	. 16

inchol-class	18
income	19
inlearn	20
ipop	22
ipop-class	24
kcca	25
kcca-class	27
kernel-class	28
kernelMatrix	29
kfa	31
kfa-class	33
kha	34
kha-class	36
kkmeans	38
kmmd	40
kmmd-class	43
kpca	44
kpca-class	47
kqr	48
kqr-class	
ksvm	
ksvm-class	
lssvm	
lssvm-class	
musk	
onlearn	
onlearn-class	
plot	
prc-class	
predict.gausspr	
predict.kgr	
predict.ksvm	
promotergene	
ranking	
ranking-class	
reuters	
rvm	
rvm-class	
sigest	88
spam	
specc	
spece-class	
spirals	· · 93 · · 94
spirals	
ticdata	· · 95
vm-class	· · 90 · · 99
viii-Class	

Index

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

х	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

Examples

```
## 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")</pre>
```

svp2

couple

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 primitive 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 csi

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

х	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

		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.
		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)
	delta	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 than 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
truegain	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))

csi-class

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))</pre>
ymat <- matrix(0, 150, 3)</pre>
ymat[yind==as.integer(iris[,5])] <- 1</pre>
datamatrix <- as.matrix(iris[,-5])</pre>
# initialize kernel function
rbf <- rbfdot(sigma=0.1)</pre>
rbf
Z <- csi(datamatrix,ymat, kernel=rbf, rank = 30)</pre>
dim(Z)
pivots(Z)
# calculate kernel matrix
K <- crossprod(t(Z))</pre>
# difference between approximated and real kernel matrix
(K - kernelMatrix(kernel=rbf, datamatrix))[6,]
```

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.

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

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])</pre>
```

```
# initialize kernel function
rbf <- rbfdot(sigma=0.1)
rbf</pre>
```

dots

```
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,]
```

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') = < x, x' >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 $k(x, x') = (-Bessel_{(\nu+1)}^n \sigma ||x - x'||^2)$ 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 $\prod_{d=1}^D 1 + x_i x_j + x_i x_j min(x_i, x_j) - \frac{x_i + x_j}{2} min(x_i, x_j)^2 + \frac{min(x_i, x_j)^3}{3}$ \ The 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

9

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

gausspr

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

X	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).

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 functionbesseldot 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	

gausspr

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

Examples

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

```
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)</pre>
# 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)</pre>
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", \ldots). or by calling the gausspr function

14

gausspr-class

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)

inchol

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

х	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

16

	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.
tol	algorithm stops when remaining pivots bring less accuracy then tol (default: 0.001)
maxiter	maximum number of iterations and columns in Z
blocksize	add this many columns to matrix per iteration
verbose	print info on algorithm convergence

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 than 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

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

18

income

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

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

	 anovadot ANOVA RBF kernel function
	The kernel parameter can also be set to a user defined function of class ker by passing the function name as an argument.
kpar	the list of hyper-parameters (kernel parameters). This is a list which contains parameters to be used with the kernel function. For valid parameters for exist kernels are :
	 sigma inverse kernel width for the Radial Basis kernel function "rbfd 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 rameter as well.
type	the type of problem to be learned by the online algorithm : classificati regression, 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

Examples

```
on <- onlearn(on,x[i,],y[i],nu=0.03,lambda=0.1)</pre>
```

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

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 $ZZ' = H$.
А	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. ipop

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)

Alexandros Karatzoglou (based on Matlab code by Alex Smola) <alexandros.karatzoglou@ci.tuwien.ac.at>

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

Examples

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
C <- 5
rbf <- rbfdot(sigma = 0.1)</pre>
## create H matrix etc.
H <- kernelPol(rbf,x,,y)</pre>
c <- matrix(rep(-1,m))</pre>
A <- t(y)
b <- 0
l <- matrix(rep(0,m))</pre>
u <- matrix(rep(C,m))</pre>
r <- 0
sv <- ipop(c,H,A,b,l,u,r)</pre>
```

```
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

Examples

```
## 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])</pre>
```

```
y[y==2] <- -1
```

kcca

```
##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
l <- matrix(rep(0,m))
u <- 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)
```

```
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

х	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 func- tions 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.
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 \boldsymbol{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

Examples

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

kcca(x,y,ncomps=2)

kcca-class

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

Class "kcca"

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

Examples

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

kcca(x,y,ncomps=2)

kernel-class

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

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

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 $H = z_i z_j k(x_i, x_j)$, $H = z_i k_j k(x_i, y_j)$. kernelMult calculates the kernel expansion $f(x_i) = \sum_{i=1}^m z_i k(x_i, x_j)$ 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.
x	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)

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

Examples

```
## 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>
```

```
rbf
## 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

x	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 for- mula).
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

kfa

	 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.)
	. 11'4' 1

... 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>

kfa-class

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.

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

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 for- mula).
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

	 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.

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.
kha-class

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

kkmeans

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

	• 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 normal- ized 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.
р	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.

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)
```

kmmd

Kernel Maximum Mean Discrepancy.

Description

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

kmmd

Usage

```
## S4 method for signature 'matrix'
kmmd(x, y, kernel="rbfdot",kpar="automatic", alpha = 0.05,
    asymptotic = FALSE, replace = TRUE, ntimes = 150, frac = 1, ...)
## S4 method for signature 'kernelMatrix'
kmmd(x, y, Kxy, alpha = 0.05,
    asymptotic = FALSE, replace = TRUE, ntimes = 100, frac = 1, ...)
## S4 method for signature 'list'
kmmd(x, y, kernel="stringdot",
    kpar = list(type = "spectrum", length = 4), alpha = 0.05,
    asymptotic = FALSE, replace = TRUE, ntimes = 150, frac = 1, ...)
```

Arguments

data values, in a matrix, list, or kernelMatrix
data values, in a matrix, list, or kernelMatrix
kernlMatrix between x and y values (only for the kernelMatrix interface)
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.
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 normal- ized 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 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 :

HØ	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

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

Description

The Kernel Maximum Mean Discrepancy object class

Class "kqr"

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

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, ...)
```

44

kpca

Arguments

8	
x	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 for- mula).
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. 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.

рсv	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

46

kpca-class

```
#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

Examples

```
kqr
```

Kernel Quantile Regression.

Description

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

Usage

```
## S4 method for signature 'formula'
kqr(x, data=NULL, ..., subset, na.action = na.omit, scaled = TRUE)
## S4 method for signature 'vector'
kqr(x,...)
## S4 method for signature 'matrix'
kqr(x, y, scaled = TRUE, tau = 0.5, C = 0.1, kernel = "rbfdot",
    kpar = "automatic", reduced = FALSE, rank = dim(x)[1]/6,
    fit = TRUE, cross = 0, na.action = na.omit)
## S4 method for signature 'kernelMatrix'
kqr(x, y, tau = 0.5, C = 0.1, fit = TRUE, cross = 0)
## S4 method for signature 'list'
kqr(x, y, tau = 0.5, C = 0.1, kernel = "strigdot",
    kpar = list(length=4, C=0.5), fit = TRUE, cross = 0)
```

Arguments

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.

48

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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)
C	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 normal- ized 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").
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

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 <- sort(runif(300))</pre>
y <- sin(pi*x) + rnorm(300,0,sd=exp(sin(2*pi*x)))</pre>
# 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 <- kqr(x, y, tau = 0.9, kernel = "rbfdot",</pre>
           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

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 kqr type: Inherited from class vm, not used in kqr

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 = "kqr"): returns the fitted values kcall signature(object = "kqr"): 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 response matrix used scaling signature(object = "kqr"): returns the response matrix used scaling signature(object = "kqr"): returns the scaling coefficients of the data (when scaled = TRUE is used)

ksvm

Author(s)

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

See Also

kqr, vm-class, ksvm-class

Examples

```
# create data
x \le sort(runif(300))
y <- sin(pi*x) + rnorm(300,0,sd=exp(sin(2*pi*x)))</pre>
# 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 <- kqr(x, y, tau = 0.9, kernel = "rbfdot",</pre>
           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
	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	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.

55

	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").
С	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 components 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

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

ksvm

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 regression, 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

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- 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.

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versity of London, Department of Computer Science.

See Also

predict.ksvm,ksvm-class,couple

Examples

```
## simple example using the spam data set
data(spam)
```

```
## create test and training set
index <- sample(1:dim(spam)[1])
spamtrain <- spam[index[1:floor(dim(spam)[1]/2)], ]
spamtest <- spam[index[((ceiling(dim(spam)[1]/2)) + 1):dim(spam)[1]], ]</pre>
```

```
filter
```

```
## predict mail type on the test set
mailtype <- predict(filter,spamtest[,-58])</pre>
```

ksvm

```
## 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 <- matrix(c(rep(1,60),rep(-1,60)))</pre>
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 <- function(x,y) {(sum(x*y) +1)*exp(-0.001*sum((x-y)^2))}</pre>
class(k) <- "kernel"</pre>
```

ksvm-class

```
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)</pre>
# train support vector machine
regm <- ksvm(x,y,epsilon=0.01,kpar=list(sigma=16),cross=3)</pre>
plot(x,y,type="1")
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

type: Object of class "character" containing the support vector machine type ("C-svc", "nu-svc", "C-bsvc", "spoc-svc", "one-svc", "eps-svr", "nu-svr", "eps-bsvr")

param: Object of class "list" containing the Support Vector Machine parameters (C, nu, epsilon)

kernelf: Object of class "function" containing the kernel function

kpar: Object of class "list" containing the kernel function parameters (hyperparameters)

kcall: Object of class "ANY" containing the ksvm function call

scaling: Object of class "ANY" containing the scaling information performed on the data

ksvm-class

- 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 classification 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 problem 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 oneagainst-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 vectors)

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

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)
```

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)
```

Description

The lssvm function is an implementation of the Least Squares SVM. lssvm 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

х	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.
data	an optional data frame containing the variables in the model. By default the variables are taken from the environment which 'lssvm' 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 classification or regression - currently nor supported -).

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.
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 normal- ized a logical parameter determining if the kernel evaluations should be normalized. Hyper-parameters for user defined kernels can be passed through the kpar pa- rameter 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").

lssvm

tau	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 decomposed 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 leastsquares 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 "lssvm" 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>

lssvm-class

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

66

lssvm-class

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 type of problem scaling signature(object = "lssvm"): returns the scaling values xmatrix signature(object = "lssvm"): returns the scaling values

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

68

onlearn

Source

UCI Machine Learning data repository

Examples

```
data(musk)
```

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

muskm

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 +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.

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

sign(predict(on,x))

onlearn-class Class "onlearn"

Description

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

onlearn-class

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 "numeric" containing the model parameters rho: Object of class "numeric" containing model parameter b: Object of class "numeric" used for dealing with factors type: 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(object = "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

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

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

predict.gausspr

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 values 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 regression.
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

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 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
- 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

Examples

```
predict.kqr
```

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>

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

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.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.

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

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
У	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.
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. 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.
If TRUE the data matrix columns are scaled to zero mean and unit variance.
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.
Maximum number of iterations
Construct edgegraph (only supported with the RBF kernel)
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

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)

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reuters

See Also

ranking

Examples

data(spirals)

create data set to be ranked
ran<-spirals[rowSums(abs(spirals)<0.55)==2,]</pre>

ranked
edgegraph(ranked)[1:10,1:10]

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

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

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

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.

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

kpar

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)</pre>
```

train relevance vector machine

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

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 calculated variance (in regression)
type signature(object = "rvm"): returns the type of problem
xmatrix signature(object = "rvm"): returns the used response

Author(s)

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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>
```

```
sigest
```

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.

spam

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 Statitiscal 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]
s
## 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.

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 ';', '(', '[', '!', '\$', 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.

specc

Usage

```
## S4 method for signature 'formula'
specc(x, data = NULL, na.action = na.omit, ...)
## S4 method for signature 'matrix'
specc(x, centers,
    kernel = "rbfdot", kpar = "automatic",
    nystrom.red = FALSE, nystrom.sample = dim(x)[1]/6,
    iterations = 200, mod.sample = 0.75, na.action = na.omit, ...)
## S4 method for signature 'kernelMatrix'
specc(x, centers, nystrom.red = FALSE, iterations = 200, ...)
## S4 method for signature 'list'
specc(x, centers,
    kernel = "stringdot", kpar = list(length=4, lambda=0.5),
    nystrom.red = FALSE, nystrom.sample = length(x)/6,
    iterations = 200, mod.sample = 0.75, na.action = na.omit, ...)
```

Arguments

X	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 de- fault character string "automatic" uses a heuristic to determine a suitable value for the width parameter of the RBF kernel. The second option "local" (local

	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 mul- tiple 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 normal- ized 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 nystrom 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

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)

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.

Methods

```
centers signature(object = "specc"): returns the cluster centers
```

```
withinss signature(object = "specc"): returns the within-cluster sum of squares for each clus-
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)</pre>

centers(sc)
size(sc)

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

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.).

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)</pre>

sk

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

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 Subtype
2	MAANTHUI	Number of houses 1 - 10
3	MGEMOMV	Avg size household 1 - 6
4	MGEMLEEF	Average age
5	MOSHOOFD	
6	MGODRK	Customer main type Roman catholic
7	MGODRR	Protestant
8	MGODPR	
		Other religion
9	MGODGE	No religion
10	MRELGE	Married
11	MRELSA	Living together
12	MRELOV	Other relation
13	MFALLEEN	Singles
14	MFGEKIND	Household without children
15	MFWEKIND	Household with children
16	MOPLHOOG	High level education
17	MOPLMIDD	Medium level education
18	MOPLLAAG	Lower level education
19	MBERHOOG	High status
20	MBERZELF	Entrepreneur
21	MBERBOER	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

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
66	AWABEDR	Number of third party insurance (firms)
67	AWALAND	Number of third party insurance (agriculture)
68	APERSAUT	Number of car policies
69	ABESAUT	Number of delivery van policies
70	AMOTSCO	Number of motorcycle/scooter policies
71	AVRAAUT	Number of lorry policies
72	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

84 AINBOED Number of property insurance policies

vm-class

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 Peter van der Putten Sentient Machine Research Baarsjesweg 224 1058 AA Amsterdam The Netherlands +31 20 6186927 pvdputten@hotmail.com, putten@liacs.nl

References

Peter van der Putten, Michel de Ruiter, Maarten van Someren *CoIL 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.

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

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See Also

ksvm-class, rvm-class, gausspr-class

Index

* algebra csi,5 inchol, 16 kernelMatrix, 29 * array csi,5 inchol, 16 kernelMatrix, 29 * classes csi-class, 7 gausspr-class, 14 inchol-class, 18 ipop-class, 24 kcca-class, 27 kernel-class, 28 kfa-class, 33 kha-class, 36 kmmd-class, 43 kpca-class, 47 kqr-class, 51 ksvm-class, 60 lssvm-class, 66 onlearn-class, 70 prc-class, 73 ranking-class, 81 rvm-class, 86 specc-class, 93 vm-class, 99 * classif couple, 4 gausspr, 11 inlearn, 20 ksvm, 53 lssvm, 63 onlearn, 69 plot, 72 predict.gausspr, 74 predict.ksvm, 76 ranking, 78

sigest, 88 * cluster kfa, <mark>31</mark> kha, 34 kkmeans, 38 kpca, 44 ranking, 78 specc, 90 * datasets income. 19 musk, 68 promotergene, 77 reuters, 82 spam, 89 spirals, 94 ticdata, 96 * htest kmmd, 40 * methods as.kernelMatrix, 3 csi, 5 gausspr, 11 inchol, 16 kgr. 48 ksvm, 53 lssvm, 63 plot, 72 predict.gausspr, 74 predict.kqr,75 predict.ksvm, 76 * multivariate kcca. 25 * neural inlearn, 20 ksvm, 53 onlearn, 69 * nonlinear gausspr, 11 kmmd, 40

```
kgr, 48
    ksvm, 53
    lssvm, 63
    rvm, 83
* nonparametric
    kmmd, 40
* optimize
    ipop, 22
* regression
    gausspr, 11
    inlearn, 20
    kgr, 48
    ksvm, 53
    onlearn, 69
    plot, 72
    predict.gausspr, 74
    predict.kqr, 75
    predict.ksvm, 76
    rvm, 83
    sigest, 88
* symbol math
    dots, 9
    stringdot, 95
* ts
    inlearn, 20
    onlearn. 69
alpha (vm-class), 99
alpha, gausspr-method (gausspr-class), 14
alpha, kfa-method (kfa-class), 33
alpha,kgr-method (kgr-class), 51
alpha,ksvm-method (ksvm-class), 60
alpha, lssvm-method (lssvm-class), 66
alpha, onlearn-method (onlearn-class), 70
alpha, rvm-method (rvm-class), 86
alpha, vm-method (vm-class), 99
alphaindex (ksvm-class), 60
alphaindex, gausspr-method
        (gausspr-class), 14
alphaindex, kfa-method (kfa-class), 33
alphaindex, kqr-method (kqr-class), 51
alphaindex, ksvm-method (ksvm-class), 60
alphaindex,lssvm-method(lssvm-class),
        66
anovadot (dots), 9
anovakernel-class (kernel-class), 28
as.kernelMatrix, 3
as.kernelMatrix,matrix-method
        (as.kernelMatrix), 3
```

as.kernelMatrix-methods (as.kernelMatrix), 3 Asymbound (kmmd), 40 Asymbound, kmmd-method (kmmd-class), 43 AsympH0 (kmmd), 40 AsympH0, kmmd-method (kmmd-class), 43 b(ksvm-class), 60 b,kgr-method(kgr-class), 51 b,ksvm-method (ksvm-class), 60 b,lssvm-method (lssvm-class), 66 b, onlearn-method (onlearn-class), 70 besseldot (dots), 9 besselkernel-class (kernel-class), 28 buffer (onlearn-class), 70 buffer, onlearn-method (onlearn-class), 70

cancor, 26 centers (specc-class), 93 centers, specc-method (specc-class), 93 chol, 7, 18 coef, gausspr-method (gausspr), 11 coef, kfa-method (kfa), 31 coef, kqr-method (kqr), 48 coef,ksvm-method(ksvm),53 coef, lssvm-method (lssvm), 63 coef, rvm-method (rvm), 83 coef, vm-method (ksvm-class), 60 convergence (ranking-class), 81 convergence, ranking-method (ranking-class), 81 couple, 4, 58 cross (vm-class), 99 cross, gausspr-method (gausspr-class), 14 cross, kqr-method (kqr-class), 51 cross,ksvm-method(ksvm-class),60 cross, lssvm-method (lssvm-class), 66 cross, rvm-method (rvm-class), 86 cross, vm-method (vm-class), 99 csi, 5, 8, 18, 19, 23, 65, 66 csi, matrix-method (csi), 5 csi-class, 7 csi-methods (csi), 5

INDEX

```
dots, 3, 9, 28, 96
dual (ipop-class), 24
dual, ipop-method (ipop-class), 24
edgegraph (ranking-class), 81
edgegraph, ranking-method
        (ranking-class), 81
eig (prc-class), 73
eig, kha-method (kha-class), 36
eig, kpca-method (kpca-class), 47
eig, prc-method (prc-class), 73
error (vm-class), 99
error, gausspr-method (gausspr-class), 14
error, kqr-method (kqr-class), 51
error, ksvm-method (ksvm-class), 60
error, lssvm-method (lssvm-class), 66
error, rvm-method (rvm-class), 86
error, vm-method (vm-class), 99
eskm, kha-method (kha-class), 36
fit, onlearn-method (onlearn-class), 70
fitted, ksvm-method (ksvm-class), 60
fitted, vm-method (vm-class), 99
fourierdot (dots), 9
fourierkernel-class (kernel-class), 28
gausspr, 11, 16, 66
gausspr, formula-method (gausspr), 11
gausspr, matrix-method (gausspr), 11
gausspr, vector-method (gausspr), 11
gausspr-class, 14
H0 (kmmd), 40
H0, kmmd-method (kmmd-class), 43
how (ipop-class), 24
how, ipop-method (ipop-class), 24
inchol, 7, 16, 19, 23
inchol, matrix-method (inchol), 16
inchol-class, 18
income, 19
inlearn, 20, 70, 71
inlearn, numeric-method (inlearn), 20
ipop, 22, 24, 51
ipop,ANY,matrix-method(ipop), 22
ipop-class, 24
```

kcall(vm-class), 99
kcall,gausspr-method(gausspr-class), 14
kcall,kfa-method(kfa-class), 33

kcall, kha-method (kha-class), 36 kcall, kpca-method (kpca-class), 47 kcall, kgr-method (kgr-class), 51 kcall,ksvm-method(ksvm-class),60 kcall,lssvm-method(lssvm-class),66 kcall, prc-method (prc-class), 73 kcall, rvm-method (rvm-class), 86 kcall, vm-method (vm-class), 99 kcca, 25, 27, 36, 40, 46, 93 kcca, matrix-method (kcca), 25 kcca-class, 27 kcor (kcca-class), 27 kcor, kcca-method (kcca-class), 27 kernel-class, 28 kernelf (vm-class), 99 kernelf, gausspr-method (gausspr-class), 14 kernelf, kfa-method (kfa-class), 33 kernelf, kha-method (kha-class), 36 kernelf, kmmd-method (kmmd-class), 43 kernelf, kpca-method (kpca-class), 47 kernelf, kgr-method (kgr-class), 51 kernelf, ksvm-method (ksvm-class), 60 kernelf, lssvm-method (lssvm-class), 66 kernelf, onlearn-method (onlearn-class). 70 kernelf, prc-method (prc-class), 73 kernelf, rvm-method (rvm-class), 86 kernelf, specc-method (specc-class), 93 kernelf, vm-method (vm-class), 99 kernelFast (kernelMatrix), 29 kernelFast, anovakernel-method (kernelMatrix), 29 kernelFast, besselkernel-method (kernelMatrix), 29 kernelFast, kernel-method (kernelMatrix), 29 kernelFast,laplacekernel-method (kernelMatrix), 29 kernelFast, polykernel-method (kernelMatrix), 29 kernelFast, rbfkernel-method (kernelMatrix), 29 kernelFast, splinekernel-method (kernelMatrix), 29 kernelFast, stringkernel-method (kernelMatrix), 29 kernelFast, tanhkernel-method

(kernelMatrix), 29 kernelFast, vanillakernel-method (kernelMatrix), 29 kernelMatrix, 3, 10, 29, 96 kernelMatrix, anovakernel-method (kernelMatrix), 29 kernelMatrix, besselkernel-method (kernelMatrix), 29 kernelMatrix, kernel-method (kernelMatrix), 29 kernelMatrix, laplacekernel-method (kernelMatrix), 29 kernelMatrix, polykernel-method (kernelMatrix), 29 kernelMatrix, rbfkernel-method (kernelMatrix), 29 kernelMatrix, splinekernel-method (kernelMatrix), 29 kernelMatrix, stringkernel-method (kernelMatrix), 29 kernelMatrix, tanhkernel-method (kernelMatrix), 29 kernelMatrix, vanillakernel-method (kernelMatrix), 29 kernelMatrix-class (as.kernelMatrix), 3 kernelMult. 10.96 kernelMult (kernelMatrix), 29 kernelMult, anovakernel, ANY-method (kernelMatrix), 29 kernelMult, besselkernel, ANY-method (kernelMatrix), 29 kernelMult, character, kernelMatrix-method (kernelMatrix), 29 kernelMult,kernel-method (kernelMatrix), 29 kernelMult, laplacekernel, ANY-method (kernelMatrix), 29 kernelMult, polykernel, ANY-method (kernelMatrix), 29 kernelMult, rbfkernel, ANY-method (kernelMatrix), 29 kernelMult, splinekernel, ANY-method (kernelMatrix), 29 kernelMult, stringkernel, ANY-method (kernelMatrix), 29 kernelMult,tanhkernel,ANY-method (kernelMatrix), 29 kernelMult, vanillakernel, ANY-method

(kernelMatrix), 29 kernelPol, 10, 96 kernelPol (kernelMatrix), 29 kernelPol, anovakernel-method (kernelMatrix), 29 kernelPol, besselkernel-method (kernelMatrix), 29 kernelPol, kernel-method (kernelMatrix), 29 kernelPol,laplacekernel-method (kernelMatrix), 29 kernelPol, polykernel-method (kernelMatrix), 29 kernelPol, rbfkernel-method (kernelMatrix), 29 kernelPol, splinekernel-method (kernelMatrix), 29 kernelPol, stringkernel-method (kernelMatrix), 29 kernelPol,tanhkernel-method (kernelMatrix), 29 kernelPol, vanillakernel-method (kernelMatrix), 29 kernels, 34, 55 kernels (dots), 9 kfa, 26, 31, 34, 36 kfa, formula-method (kfa), 31 kfa, matrix-method (kfa), 31 kfa-class, 33 kfunction (dots), 9 kfunction-class (kernel-class), 28 kha, 26, 34, 37 kha, formula-method (kha), 34 kha, matrix-method (kha), 34 kha-class, 36 kkmeans, 38, 93 kkmeans, formula-method (kkmeans), 38 kkmeans, kernelMatrix-method (kkmeans), 38 kkmeans, list-method (kkmeans), 38 kkmeans, matrix-method (kkmeans), 38 kmmd, 40, 44 kmmd, kernelMatrix-method (kmmd), 40 kmmd,list-method(kmmd),40 kmmd, matrix-method (kmmd), 40 kmmd-class, 43 kpar (dots), 9 kpar, gausspr-method (gausspr-class), 14

INDEX

kpar, kernel-method (kernel-class), 28 kpar, kqr-method (kqr-class), 51 kpar, ksvm-method (ksvm-class), 60 kpar, lssvm-method (lssvm-class), 66 kpar, onlearn-method (onlearn-class), 70 kpar, rvm-method (rvm-class), 86 kpar, vm-method (vm-class), 99 kpca, 26, 33, 36, 40, 44, 93 kpca, formula-method (kpca), 44 kpca, kernelMatrix-method (kpca), 44 kpca, list-method (kpca), 44 kpca, matrix-method (kpca), 44 kpca-class, 47 kgr, 48, 53 kqr,formula-method(kqr),48 kgr, kernelMatrix-method (kgr), 48 kqr,list-method(kqr),48 kqr, matrix-method (kqr), 48 kgr, vector-method (kgr), 48 kgr-class, 51 ksvm, 5, 13, 51, 53, 62, 66, 72, 85, 89 ksvm, formula-method (ksvm), 53 ksvm, kernelMatrix-method (ksvm), 53 ksvm,list-method(ksvm), 53 ksvm, matrix-method (ksvm), 53 ksvm, vector-method (ksvm), 53 ksvm-class, 60

```
laplacedot (dots), 9
laplacekernel-class (kernel-class), 28
lev (vm-class), 99
lev, gausspr-method (gausspr-class), 14
lev,ksvm-method (ksvm-class), 60
lev, lssvm-method (lssvm-class), 66
lev, rvm-method (rvm-class), 86
lev, vm-method (vm-class), 99
lssvm, 13, 63, 68
lssvm, formula-method (lssvm), 63
lssvm,kernelMatrix-method(lssvm), 63
lssvm,list-method(lssvm), 63
lssvm, matrix-method (lssvm), 63
lssvm,vector-method(lssvm), 63
lssvm-class, 66
lssvm-methods (lssvm), 63
```

mlike(rvm-class), 86
mlike,rvm-method(rvm-class), 86
mmdstats(kmmd), 40
mmdstats,kmmd-method(kmmd-class), 43
musk, 68

nSV (ksvm-class), 60 nSV, ksvm-method (ksvm-class), 60 nSV, lssvm-method (lssvm-class), 66 nvar (rvm-class), 86 nvar, rvm-method (rvm-class), 86

obj (ksvm-class), 60 obj, ksvm-method (ksvm-class), 60 onlearn, 21, 69, 71 onlearn, onlearn-method (onlearn), 69 onlearn-class, 70

param (ksvm-class), 60 param, kqr-method (kqr-class), 51 param, ksvm-method (ksvm-class), 60 param, lssvm-method (lssvm-class), 66 pcv (prc-class), 73 pcv, kha-method (kha-class), 36 pcv, kpca-method (kpca-class), 47 pcv, prc-method (prc-class), 73 pivots (inchol-class), 18 pivots, csi-method (csi-class), 7 pivots, inchol-method (inchol-class), 18 plot, 72 plot,ksvm,missing-method (plot), 72 plot,ksvm-method (plot), 72 plot.ksvm(plot), 72 polydot, 30 polydot (dots), 9 polykernel-class (kernel-class), 28 prc-class, 73 predgain (csi-class), 7 predgain, csi-method (csi-class), 7 predict, gausspr-method (predict.gausspr), 74 predict, kfa-method (kfa-class), 33 predict, kha-method (kha), 34 predict, kpca-method (kpca), 44 predict,kgr-method(predict.kgr),75 predict, ksvm-method (predict.ksvm), 76 predict, lssvm-method (lssvm), 63 predict,onlearn-method(onlearn-class),

```
70
```

```
predict, rvm-method (rvm), 83
predict.gausspr, 13, 74
predict.kgr, 51, 75
predict.ksvm, 5, 58, 76
primal (ipop-class), 24
primal, ipop-method (ipop-class), 24
prior (ksvm-class), 60
prior, ksvm-method (ksvm-class), 60
prob.model (ksvm-class), 60
prob.model,ksvm-method(ksvm-class), 60
promotergene, 77
Q(csi-class), 7
Q, csi-method (csi-class), 7
R(csi-class), 7
R, csi-method (csi-class), 7
Radbound (kmmd), 40
Radbound, kmmd-method (kmmd-class), 43
ranking, 78, 82
ranking, kernelMatrix-method (ranking),
        78
ranking,list-method(ranking),78
ranking,matrix-method(ranking), 78
ranking-class, 81
rbfdot, 30
rbfdot (dots). 9
rbfkernel-class (kernel-class), 28
reuters. 82
rho (onlearn-class), 70
rho, onlearn-method (onlearn-class), 70
rlabels (reuters), 82
rotated (kpca-class), 47
rotated, kpca-method (kpca-class), 47
RVindex (rvm-class), 86
RVindex, rvm-method (rvm-class), 86
rvm, 13, 51, 83, 87
rvm, formula-method (rvm), 83
rvm, kernelMatrix-method (rvm), 83
rvm,list-method(rvm),83
rvm, matrix-method (rvm), 83
rvm, vector-method (rvm), 83
rvm-class, 86
rvm-methods (rvm), 83
scaling (ksvm-class), 60
scaling,gausspr-method(gausspr-class),
         14
```

scaling,kqr-method(kqr-class),51

scaling,ksvm-method(ksvm-class),60 scaling,lssvm-method(lssvm-class),66 show (ksvm-class), 60 show, gausspr-method (gausspr), 11 show, kernel-method (dots), 9 show, kfa-method (kfa), 31 show, kmmd-method (kmmd), 40 show, kqr-method (kqr), 48 show, ksvm-method (ksvm), 53 show, lssvm-method (lssvm), 63 show, onlearn-method (onlearn-class), 70 show, ranking-method (ranking-class), 81 show, rvm-method (rvm), 83 show, specc-method (specc), 90 sigest, 56, 64, 84, 88 sigest, formula-method (sigest), 88 sigest,matrix-method(sigest), 88 size (specc-class), 93 size, specc-method (specc-class), 93 spam, 89 specc, 40, 81, 90, 94 specc, formula-method (specc), 90 specc,kernelMatrix-method(specc),90 specc,list-method(specc),90 specc, matrix-method (specc), 90 specc-class, 93 spirals, 94 splinedot(dots), 9 splinekernel-class (kernel-class), 28 stringdot, 95 stringkernel-class (kernel-class), 28 SVindex (ksvm-class), 60 SVindex, ksvm-method (ksvm-class), 60 tanhdot, 30 tanhdot (dots), 9 tanhkernel-class (kernel-class), 28 ticdata, 96 truegain (csi-class), 7 truegain,csi-method(csi-class),7

type (vm-class), 99
type,gausspr-method (gausspr-class), 14
type,ksvm-method (ksvm-class), 60
type,lssvm-method (lssvm-class), 66
type,onlearn-method (onlearn-class), 70
type,rvm-method (rvm-class), 86
type,vm-method (vm-class), 99

vanilladot, 30

INDEX

```
vanilladot (dots), 9
vanillakernel-class (kernel-class), 28
vm-class, 99
withinss (specc-class), 93
withinss, specc-method (specc-class), 93
xcoef (kcca-class), 27
xcoef,kcca-method(kcca-class), 27
xmatrix (vm-class), 99
xmatrix,gausspr-method(gausspr-class),
        14
xmatrix, kfa-method (kfa-class), 33
xmatrix, kha-method (kha-class), 36
xmatrix,kpca-method(kpca-class),47
xmatrix,kqr-method(kqr-class), 51
xmatrix,ksvm-method(ksvm-class), 60
xmatrix,lssvm-method(lssvm-class),66
xmatrix,onlearn-method(onlearn-class),
        70
xmatrix, prc-method (prc-class), 73
xmatrix,rvm-method(rvm-class),86
xmatrix,vm-method(vm-class),99
xvar,kcca-method(kcca-class), 27
ycoef (kcca-class), 27
ycoef,kcca-method(kcca-class), 27
ymatrix (vm-class), 99
ymatrix,gausspr-method(gausspr-class),
        14
ymatrix,kqr-method(kqr-class), 51
ymatrix,ksvm-method(ksvm-class),60
ymatrix,lssvm-method(lssvm-class),66
ymatrix,rvm-method (rvm-class), 86
ymatrix,vm-method (vm-class), 99
yvar, kcca-method (kcca-class), 27
```