Package ‘qkerntool’

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Title Q-Kernel-Based and Conditionally Negative Definite Kernel-Based Machine Learning Tools

Version 1.19

Description Nonlinear machine learning tool for classification, clustering and dimensionality reduction. It integrates 12 q-kernel functions and 15 conditional negative definite kernel functions and includes the q-kernel and conditional negative definite kernel version of density-based spatial clustering of applications with noise, spectral clustering, generalized discriminant analysis, principal component analysis, multidimensional scaling, locally linear embedding, sammon's mapping and t-Distributed stochastic neighbor embedding.

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as.cndkernmatrix

Assing cndkernmatrix class to matrix objects

as.cndkernmatrix in package qkerntool can be used to create the cndkernmatrix class to matrix objects representing a CND kernel matrix. These matrices can then be used with the cndkernmatrix interfaces which most of the functions in qkerntool support.

Usage

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

Arguments

- `x`: matrix to be assigned the cndkernmatrix class
- `center`: center the cndkernel matrix in feature space (default: FALSE)
as.qkernmatrix

Author(s)

Yusen Zhang
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See Also

cndkernmatrix,qkernmatrix

Examples

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

### Use as.cndkernmatrix to label the cov. matrix as a CND kernel matrix
### which is eq. to using a linear kernel
K <- as.cndkernmatrix(crossprod(t(x)))
K
```

Description

as.qkernmatrix in package qkerntool can be used to create the qkernmatrix class to matrix objects representing a q kernel matrix. These matrices can then be used with the qkernmatrix interfaces which most of the functions in qkerntool support.

Usage

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

Arguments

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

Author(s)

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bases

qKernel Functions

Description

The kernel generating functions provided in qkerntool.
The Non Linear Kernel \( k(x, y) = \frac{1}{2(1-q)}(q^{-\alpha}|x|^\alpha + q^{-\alpha}|y|^\alpha - 2q^{-\alpha}x'y) \).
The Gaussian kernel \( k(x, y) = \frac{1}{1-q}(1 - q(|x-y|/\sigma)^2) \).
The Laplacian Kernel \( k(x, y) = \frac{1}{1-q}(1 - q(|x-y|/\sigma)) \).
The Rational Quadratic Kernel \( k(x, y) = \frac{1}{1-q}(1 - q|x-y|^2 + \gamma) \).
The Multiquadric Kernel \( k(x, y) = \frac{1}{1-q}(q^{-\frac{1}{2}} - q^{-\frac{1}{2}}\sqrt{|x-y|^2 + \gamma}) \).
The Inverse Multiquadric Kernel \( k(x, y) = \frac{1}{1-q}(1 - q\sqrt{|x-y|^2 + \gamma}) \).
The Wave Kernel \( k(x, y) = \frac{1}{1-q}(q^{-\frac{1}{2}} - q^{-\frac{1}{2}}\sqrt{|x-y|^2 + \gamma}) \).
The d Kernel \( k(x, y) = \frac{1}{1-q}(1 - q(|x-y|^{d/2}) \).
The Log Kernel \( k(x, y) = \frac{1}{1-q}(1 - q^\theta n(|x-y|^{d/2} + 1)) \).
The Cauchy Kernel \( k(x, y) = \frac{1}{1-q}(q^{-1} - q^{-1}|x-y|^{d/2}) \).
The Chi-Square Kernel \( k(x, y) = \frac{1}{1-q}(1 - q^{\gamma} n^2/(x+y) \).
The Generalized T-Student Kernel \( k(x, y) = \frac{1}{1-q}(1 - q^{-1} - q^{-1}|x-y|^{d/2}) \).

Usage

rbfbase(sigma = 1, q = 0.8)
nonlbase(alpha = 1, q = 0.8)
bases

```r
laplbase(sigma = 1, q = 0.8)
ratibase(c = 1, q = 0.8)
multibase(c = 1, q = 0.8)
invbase(c = 1, q = 0.8)
wavbase(theta = 1, q = 0.8)
powbase(d = 2, q = 0.8)
logbase(d = 2, q = 0.8)
caubase(sigma = 1, q = 0.8)
chibase(gamma = 1, q = 0.8)
studbase(d = 2, q = 0.8)
```

**Arguments**

- `q` for all the qkernel function.
- `sigma` for the Radial Basis qkernel function "rbfbase" , the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
- `alpha` for the Non Linear qkernel function "nonlbase".
- `c` for the Rational Quadratic qkernel function "ratibase" , the Multiquadric qkernel function "multibase" and the Inverse Multiquadric qkernel function "invbase".
- `theta` for the Wave qkernel function "wavbase".
- `d` for the d qkernel function "powbase" , the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
- `gamma` for the Chi-Square qkernel function "chibase".

**Details**

The kernel generating functions are used to initialize a kernel function which calculates the kernel function value between two feature vectors in a Hilbert Space. These functions can be passed as a qkernel argument on almost all functions in qkerntool(e.g., qkgda, qkpca etc).

**Value**

Return an S4 object of class qkernel which extents the function class. The resulting function implements the given kernel calculating the kernel function value between two vectors.

- `qpar` a list containing the kernel parameters (hyperparameters) used.

The kernel parameters can be accessed by the qpar function.

**Author(s)**

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**See Also**

qkernmatrix, cndkernmatrix
Examples

```r
qkfunc <- rbfbase(sigma=1,q=0.8)
qkfunc

qpar(qkfunc)

## create two vectors
x <- rnorm(10)
y <- rnorm(10)

## calculate dot product
qkfunc(x,y)
```

---

**blkdiag**

*Block diagonal concatenation of matrix*

---

Description

\[ Y = \text{BLKDIAG}(A,B,...) \text{ produces diag}(A,B,...) \]

Usage

```r
blkdiag(x)
```

Arguments

\( x \quad \text{a list of matrix} \)

Value

\( E \quad \text{Block diagonal concatenation of matrix} \)

Author(s)

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Description

The built-in kernel classes in qkerntool

Objects from the Class

Objects can be created by calls of the form `new("nonlkernel"), new("polykernel"), new("rbfkernel"), new("laplkernel"), new("anokernel"), new("ratikernel"), new("multkernel"), new("invkernel"), new("wavkernel"), new("powkernel"), new("logkernel"), new("caukernel"), new("chikernel"), new("studkernel"), new("norkernel")`

or by calling the `nonlcnd, polycnd, rbfcnd, laplcnd, anocnd, raticnd, multcnd, invcnd, wavcnd, powcnd, logcnd, caucnd, chicnd, studcnd, norcnd` functions etc..

Slots

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

`qpar`: Object of class "list" containing the kernel parameters

Methods

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

Author(s)

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See Also

`qkernmatrix, cndkernmatrix`

Examples

```r
    cndkfunc <- rbfcnd(gamma = 1)
cndkfunc

    qpar(cndkfunc)

    ## create two vectors
    x <- rnorm(10)
y <- rnorm(10)

    cndkfunc(x,y)
```
cndkernmatrix CND Kernel Matrix functions

Description
cndkernmatrix calculates the kernel matrix $K_{ij} = k(x_i, x_j)$ or $K_{ij} = k(x_i, y_j)$.

Usage

```r
## S4 method for signature 'cndkernel'
cndkernmatrix(cndkernel, x, y = NULL)
```

Arguments

- `cndkernel` the cndkernel function to be used to calculate the CND kernel matrix. This has to be a function of class cndkernel, i.e. which can be generated either one of the build in kernel generating functions (e.g., rbfcdnl nonlcnd etc.) or a user defined function of class cndkernel taking two vector arguments and returning a scalar.
- `x` a data matrix to be used to calculate the kernel matrix.
- `y` second data matrix to calculate the kernel matrix.

Details

Common functions used during kernel based computations.
The cndkernel parameter can be set to any function, of class cndkernel, which computes the kernel function value in feature space between two vector arguments. qkerntool provides more than 10 CND kernel functions which can be initialized by using the following functions:

- `nonlcnd` Non Linear cndkernel function
- `polyncnd` Polynomial cndkernel function
- `rbfcdnl` Gaussian cndkernel function
- `laplcdnl` Laplacian cndkernel function
- `anocnd` ANOVA cndkernel function
- `raticnd` Rational Quadratic cndkernel function
- `multcnd` Multiquadric cndkernel function
- `invcnd` Inverse Multiquadric cndkernel function
- `wavcnd` Wave cndkernel function
- `powcnd` d cndkernel function
- `logcnd` Log cndkernel function
- `caucnd` Cauchy cndkernel function
- `chicnd` Chi-Square cndkernel function
- `studcnd` Generalized T-Student cndkernel function

(see example.)
Value

cndkernmatrix returns a conditionally negative definite matrix with a zero diagonal element.

Author(s)

Yusen Zhang
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See Also

nonlbase, rbfbase, laplbase, ratibase, multibase, invbase, wavbase, powbase, logbase, caubase, chibase, studbase

Examples

```r
## use the iris data
data(iris)
dt <- as.matrix(iris[, -5])

## initialize cndkernel function
lapl <- laplcnd(gamma = 1)
lapl

## calculate cndkernel matrix
cndkernmatrix(lapl, dt)
```

Description

The kernel generating functions provided in qkerntool.
The Non Linear Kernel \( k(x, y) = \frac{\exp(\alpha \|x\|^2) + \exp(\alpha \|y\|^2) - 2\exp(\alpha x'y)}/2. \)
The Polynomial kernel \( k(x, y) = (\alpha \|x\|^2 + c)^d + (\alpha \|y\|^2 + c)^d - 2(\alpha x'y + c)^d)/2. \)
The Gaussian kernel \( k(x, y) = 1 - \exp(-\|x - y\|^2/\gamma). \)
The Laplacian Kernel \( k(x, y) = 1 - \exp(-\|x - y\|/\gamma). \)
The ANOVA Kernel \( k(x, y) = n - \sum \exp(-\sigma(x - y)^2)^d. \)
The Rational Quadratic Kernel \( k(x, y) = \|x - y\|^2/(\|x - y\|^2 + c). \)
The Multiquadric Kernel \( k(x, y) = \sqrt{(\|x - y\|^2 + c^2)} - c. \)
The Inverse Multiquadric Kernel \( k(x, y) = 1/c - 1/\sqrt{\|x - y\|^2 + c^2}. \)
The Wave Kernel \( k(x, y) = 1 - \frac{\theta}{\|x - y\|^2} \sin \frac{|x - y|}{\theta}. \)
The d Kernel \( k(x, y) = \|x - y\|^d. \)
The Log Kernel \( k(x, y) = \log(\|x - y\|^d + 1). \)
The Cauchy Kernel \( k(x, y) = 1 - 1/(1 + \|x - y\|^2/\gamma). \)
The Chi-Square Kernel \( k(x, y) = \sum 2(x - y)^2/(x + y). \)
The Generalized T-Student Kernel \( k(x, y) = 1 - 1/(1 + \|x - y\|^d). \)
The normal Kernel \( k(x, y) = \|x - y\|^2. \)
Usage

nonlcnd(alpha = 1)
polynd(d = 2, alpha = 1, c = 1)
rbfnd(gamma = 1)
lplnd(gamma = 1)
anoid(d = 2, sigma = 1)
raticn(c = 1)
multnd(c = 1)
invcn(c = 1)
waivnd(theta = 1)
pownd(d = 2)
logn(d = 2)
cau(n(d = 1)
chi(n( )
studn(d = 2)
nordn()

Arguments

alpha for the Non Linear cndkernel function "nonlcnd" and the Polynomial cndkernel function "polynd".
gamma for the Radial Basis cndkernel function "rbfnd" and the Laplacian cndkernel function "lplnd" and the Cauchy cndkernel function "cau(n".
sigma for the ANOVA cndkernel function "anoid".
theta for the Wave cndkernel function "waivnd".
c for the Rational Quadratic cndkernel function "raticn", the Polynomial cndkernel function "polynd", the Multiquadric cndkernel function "multnd" and the Inverse Multiquadric cndkernel function "invcn".
d for the Polynomial cndkernel function "polynd", the ANOVA cndkernel function "anoid", the cndkernel function "pownd", the Log cndkernel function "logn" and the Generalized T-Student cndkernel function "studn".

Details

The kernel generating functions are used to initialize a kernel function which calculates the kernel function value between two feature vectors in a Hilbert Space. These functions can be passed as a qkernel argument on almost all functions in qkerntool.

Value

Return an S4 object of class cndkernel which extents the function class. The resulting function implements the given kernel calculating the kernel function value between two vectors.

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

The kernel parameters can be accessed by the qpar function.
### Eucdist

**Description**

`Eucdist` computes the Euclidean (square Euclidean) distance matrix.

**Arguments**

- `x` (NxD) matrix (N samples, D features)
- `y` (MxD) matrix (M samples, D features)
- `sEuclidean` can be TRUE or FALSE, FALSE to compute the Euclidean distance matrix.

**Value**

`E` - (MxN) Euclidean (square Euclidean) distances between vectors in `x` and `y`

**Author(s)**

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<yusenzhang@126.com>
Examples

```r
###
data(iris)
testset <- sample(1:150,20)
x <- as.matrix(iris[-testset,-5])
y <- as.matrix(iris[testset,-5])

##
res0 <- Eucdist(x)
res1 <- Eucdist(x, x, sEuclidean = FALSE)
res2 <- Eucdist(x, y = NULL, sEuclidean = FALSE)
res3 <- Eucdist(x, x, sEuclidean = TRUE)
res4 <- Eucdist(x, y = NULL)
res5 <- Eucdist(x, sEuclidean = FALSE)
```

---

**mfeat_pix**  
*mfeat_pix dataset*

Description

This dataset consists of features of handwritten numerals (‘0’–‘9’) extracted from a collection of Dutch utility maps. 200 patterns per class (for a total of 2,000 patterns) have been digitized in binary images. This dataset is about 240 pixel averages in 2 x 3 windows.

Usage

```r
data("mfeat_pix")
```

Format

A data frame with 2000 observations on the following 240 variables.

Source

https://archive.ics.uci.edu/ml/datasets/Multiple+Features

Examples

```r
data(mfeat_pix)
```
qkdbscan

qKernel-DBSCAN density reachability and connectivity clustering

Description

Similar to the Density-Based Spatial Clustering of Applications with Noise (or DBSCAN) algorithm, qKernel-DBSCAN is a density-based clustering algorithm that can be applied under both linear and non-linear situations.

Usage

```r
## S4 method for signature 'matrix'
qkdbscan(x, kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
         eps = 0.25, MinPts = 5, hybrid = TRUE, seeds = TRUE,
         showplot = FALSE, countmode = NULL, na.action = na.omit, ...)

## S4 method for signature 'cndkernmatrix'
qkdbscan(x, eps = 0.25, MinPts = 5, seeds = TRUE,
         showplot = FALSE, countmode = NULL, ...)

## S4 method for signature 'qkernmatrix'
qkdbscan(x, eps = 0.25, MinPts = 5, seeds = TRUE,
         showplot = FALSE, countmode = NULL, ...)

## S4 method for signature 'qkdbscan'
predict(object, data, newdata = NULL, predict.max = 1000, ...)
```

Arguments

- **x**
  - the data matrix indexed by row, or a kernel matrix of `cndkernmatrix` or `qkernmatrix`.
- **kernel**
  - the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. `qkerntool` provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:
    - `rbfbase` Radial Basis qkernel function "Gaussian"
    - `nonlbase` Non Linear qkernel function
    - `laplbase` Laplace qkernel function
    - `ratibase` Rational Quadratic qkernel function
    - `multbase` Multiqadric qkernel function
    - `invbase` Inverse Multiqadric qkernel function
    - `wavbase` Wave qkernel function
    - `powbase` Power qkernel function
    - `logbase` Log qkernel function
    - `caubase` Cauchy qkernel function
• chibase Chi-Square qkernel function
• studbase Generalized T-Student qkernel function
• nonlcnd Non Linear cndkernel function
• polycnd Polynomial cndkernel function
• rbfcnd Radial Basis cndkernel function "Gaussian"
• laplcnd Laplacian cndkernel function
• anocnd ANOVA cndkernel function
• raticnd Rational Quadratic cndkernel function
• multcnd Multiquadric cndkernel function
• invcnd Inverse Multiquadric cndkernel function
• wavcnd Wave cndkernel function
• powcnd Power cndkernel function
• logcnd Log cndkernel function
• caucnd Cauchy cndkernel function
• studcnd Generalized T-Student cndkernel function

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

qpar 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, q for the Radial Basis qkernel function "rbfbase", the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
• alpha, q for the Non Linear qkernel function "nonlbase".
• c, q for the Rational Quadratic qkernel function "ratibase", the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
• theta, q for the Wave qkernel function "wavbase".
• d, q for the Power qkernel function "powbase", the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
• alpha for the Non Linear cndkernel function "nonlcnd".
• power, alpha, c for the Polynomial cndkernel function "polycnd".
• gamma for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
• power, sigma for the ANOVA cndkernel function "anocnd".
• c for the Rational Quadratic cndkernel function "raticnd", the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
• theta for the Wave cndkernel function "wavcnd".
• power for the Power cndkernel function "powcnd", the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

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

eps
reachability distance, see Ester et al. (1996). (default: 0.25)
MinPts
reachability minimum number of points, see Ester et al. (1996). (default: 5)
hybrid
whether the algorithm expects raw data but calculates partial distance matrices, can be TRUE or FALSE
seeds
can be TRUE or FALSE. FALSE to not include the iseseed-vector in the dbscan-object.
showplot
whether to show the plot or not, can be TRUE or 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.)
countmode
NULL or vector of point numbers at which to report progress.
object
object of class dbscan.
data
matrix or data.frame.
newdata
matrix or data.frame with raw data to predict.
predict.max
max. batch size for predictions.
...
Further arguments transferred to plot methods.

Details
The data can be passed to the qkdbscan function in a matrix, in addition qkdbscan also supports input in the form of a kernel matrix of class qkernmatrix or class cndkernmatrix.

Value
predict(qkdbscan-method) gives out a vector of predicted clusters for the points in newdata.
qkdbscan gives out an S4 object which is a LIST with components
clust
integer vector coding cluster membership with noise observations (singletons) coded as 0
eps
parameter eps
MinPts
parameter MinPts
kcall
the function call
cndkernf
the kernel function used
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)
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qkdbscan-class

References

Martin Ester, Hans-Peter Kriegel, Joerg Sander, Xiaowei Xu(1996). *A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise* Institute for Computer Science, University of Munich. *Proceedings of 2nd International Conference on Knowledge Discovery and Data Mining (KDD-96)*

See Also

qkernmatrix, cndkernmatrix

Examples

```r
# a simple example using the iris
data(iris)
test <- sample(1:150,20)
x <- as.matrix(iris[-test,-5])
ds <- qkdbscan(x, kernel="laplbase", qpar=list(sigma=3.5, q=0.8), eps=0.15, MinPts=5, hybrid = FALSE)
plot(ds, x)
emb <- predict(ds, x, as.matrix(iris[test,-5]))
points(iris[test,], col= as.integer(1+emb))
```

qkdbscan-class  

Class "qkdbscan"

Description

The qkernel-DBSCAN class.

Objects of class "qkdbscan"

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

Slots

- **clust**: Object of class "vector" containing the cluster membership of the samples
- **eps**: Object of class "numeric" containing the reachability distance
- **MinPts**: Object of class "numeric" containing the reachability minimum number of points
- **isseed**: Object of class "logical" containing the logical vector indicating whether a point is a seed (not border, not noise)
qkernel-class

Methods

- **clust** signature(object = "qkdbscan"): returns the cluster membership
- **kcall** signature(object = "qkdbscan"): returns the performed call
- **cndkernf** signature(object = "qkdbscan"): returns the used kernel function
- **eps** signature(object = "qkdbscan"): returns the reachability distance
- **MinPts** signature(object = "qkdbscan"): returns the reachability minimum number of points
- **predict** signature(object = "qkdbscan"): embeds new data
- **xmatrix** signature(object = "qkdbscan"): returns the used data matrix

Author(s)

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See Also

- qkernel-class, cndkernel-class

Examples

```r
# a simple example using the iris data
x <- as.matrix(iris[, -5])
ds <- qkdbscan (x, kernel="laplbase", qpar=list(sigma=3.5,q=0.8), eps=0.15,
MinPts=5, hybrid = FALSE)
# print the results
clust(ds)
eps(ds)
MinPts(ds)
cndkernf(ds)
xmatrix(ds)
kcall(ds)
```

Description

The built-in kernel classes in qkerntool
Objects from the Class

Objects can be created by calls of the form `new("rbfqkernel")`, `new("nonlqkernel")`, `new("laplqkernel")`, `new("ratiqkernel")`, `new("multqkernel")`, `new("invqkernel")`, `new("wavqkernel")`, `new("powqkernel")`, `new("logqkernel")`, `new("cauqkernel")`, `new("chiqkernel")`, `new("studqkernel")`

or by calling the `rbfbase`, `nonlbase`, `laplbase`, `ratibase`, `multbase`, `invbase`, `wavbase`, `powbase`, `logbase`, `caubase`, `chibase`, `studbase` functions etc..

Slots

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

Methods

qkernmatrix signature(kernel = "rbfqkernel", x = "matrix"): computes the qkernel matrix

Author(s)

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See Also

qkernmatrix, cndkernmatrix

Examples

```r
qfunc <- rbfbase(sigma=1, q=0.8)
qfunc
qpar(qfunc)

## create two vectors
x <- rnorm(10)
y <- rnorm(10)

## calculate dot product
qfunc(x, y)
```

qkernmatrix  qKernel Matrix functions

Description

qkernmatrix calculates the qkernel matrix $K_{ij} = k(x_i, x_j)$ or $K_{ij} = k(x_i, y_j)$. 
## Usage

```r
## S4 method for signature 'qkernel'
qkernmatrix(qkernel, x, y = NULL)
```

### Arguments

- **qkernel**: the kernel function to be used to calculate the qkernel matrix. This has to be a function of class `qkernel`, i.e. which can be generated either one of the build in kernel generating functions (e.g., `rbfbase` etc.) or a user defined function of class `qkernel` taking two vector arguments and returning a scalar.
- **x**: a data matrix to be used to calculate the kernel matrix
- **y**: second data matrix to calculate the kernel matrix

### Details

Common functions used during kernel based computations. The `qkernel` parameter can be set to any function, of class `qkernel`, which computes the kernel function value in feature space between two vector arguments. `qkerntool` provides more than 10 `qkernel` functions which can be initialized by using the following functions:

- `nonlbase`: Non Linear qkernel function
- `rbfbase`: Gaussian qkernel function
- `laplbase`: Laplacian qkernel function
- `ratibase`: Rational Quadratic qkernel function
- `multbase`: Multiquadric qkernel function
- `invbase`: Inverse Multiquadric qkernel function
- `wavbase`: Wave qkernel function
- `powbase`: Power qkernel function
- `logbase`: Log qkernel function
- `caubase`: Cauchy qkernel function
- `chibase`: Chi-Square qkernel function
- `studbase`: Generalized T-Student qkernel function

(see example.)

### Value

`qkernmatrix` returns a conditionally negative definite matrix with a zero diagonal element.

### Author(s)

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See Also

nonlcnd, rbfcnd, polycnd, laplcnd, anocnd, raticnd, multcnd, invcnd, wavcnd, powcnd, logcnd, caucnd, chicnd, studcnd

Examples

data(iris)
dt <- as.matrix(iris[, -5])

## initialize kernel function
rbf <- rbfbase(sigma = 1.4, q=0.8)
rbf

## calculate qkernel matrix
qkernmatrix(rbf, dt)

qkkgda

qKernel Generalized Discriminant Analysis

Description

The qkernel Generalized Discriminant Analysis is a method that deals with nonlinear discriminant analysis using kernel function operator.

Usage

## S4 method for signature 'matrix'
qkgda(x, label, kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
  features = 0, th = 1e-4, na.action = na.omit, ...)

## S4 method for signature 'cndkernmatrix'
qkgda(x, label, features = 0, th = 1e-4, na.action = na.omit, ...)

## S4 method for signature 'qkernmatrix'
qkgda(x, label, features = 0, th = 1e-4, ...)

Arguments

x the data matrix indexed by row, or a kernel matrix of cndkernmatrix or qkernmatrix.
label The original labels of the samples.
kernelfthe kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. qkerntool provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:
  • rbfbase Radial Basis qkernel function “Gaussian”

qkgda
• nonlbase Non Linear qkernel function
• laplbase Laplace qkernel function
• ratibase Rational Quadratic qkernel function
• multbase Multiquadric qkernel function
• invbase Inverse Multiquadric qkernel function
• wavbase Wave qkernel function
• powbase Power qkernel function
• logbase Log qkernel function
• caubase Cauchy qkernel function
• chibase Chi-Square qkernel function
• studbase Generalized T-Student qkernel function
• nonlcnd Non Linear cndkernel function
• polycnd Polynomial cndkernel function
• rbfcnd Radial Basis cndkernel function "Gaussian"
• laplcnd Laplacian cndkernel function
• anocnd ANOVA cndkernel function
• raticnd Rational Quadratic cndkernel function
• multcnd Multiquadric cndkernel function
• invcnd Inverse Multiquadric cndkernel function
• wavcnd Wave cndkernel function
• powcnd Power cndkernel function
• logcnd Log cndkernel function
• caucnd Cauchy cndkernel function
• chicnd Chi-Square cndkernel function
• studcnd Generalized T-Student cndkernel function

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, q for the Radial Basis qkernel function "rbfbase", the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
• alpha, q for the Non Linear qkernel function "nonlbase".
• c, q for the Rational Quadratic qkernel function "ratibase", the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
• theta, q for the Wave qkernel function "wavbase".
• d, q for the Power qkernel function "powbase", the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
• alpha for the Non Linear cndkernel function "nonlcnd".
• d, alpha, c for the Polynomial cndkernel function "polycnd".
• gamma for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
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

The qkernel Generalized Discriminant Analysis method provides a mapping of the input vectors into high dimensional feature space, generalizing the classical Linear Discriminant Analysis to non-linear discriminant analysis.

The data can be passed to the qkgda function in a matrix, in addition qkgda also supports input in the form of a kernel matrix of class qkernmatrix or class cndkernmatrix.

Value

An S4 object containing the eigenvectors and their normalized projections, along with the corresponding eigenvalues and the original function.

prj The normalized projections on eigenvectors

eVal The corresponding eigenvalues

eVec The corresponding eigenvectors

kcall The formula of the function called

ckernf The kernel function used

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)

Yusen Zhang
<yusenzhang@126.com>
References

2. Deng Cai, Xiaofei He, and Jiawei Han: Speed Up Kernel Discriminant Analysis. The VLDB Journal, January, 2011, vol.20, no.1, 21-33.

See Also

qkernmatrix, cndkernmatrix

Examples

```r
Iris <- data.frame(rbind(iris3[,1], iris3[,2], iris3[,3]), Sp = rep(c("1","2","3"), rep(50,3)))
testset <- sample(1:150,20)
train <- as.matrix(iris[-testset,-5])
test <- as.matrix(iris[testset,-5])
Sp = rep(c("1","2","3"), rep(50,3))
labels <- as.numeric(Sp)
trainlabel <- labels[-testset]
testlabel <- labels[testset]

kgda1 <- qkgda(train, label=trainlabel, kernel = "ratibase", qpar = list(c=1,q=0.9), features = 2)

prj(kgda1)
eVal(kgda1)
eVec(kgda1)
kcall(kgda1)
# xmatrix(kgda1)

# print the principal component vectors
prj(kgda1)
# plot the data projection on the components
plot(kgda1@prj,col=as.integer(train), xlab="1st Principal Component",ylab="2nd Principal Component")
```

qkgda-class

Class "qkgda"

Description

The qkernel Generalized Discriminant Analysis class

Objects of class "qkgda"

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

- **prj**: Object of class "matrix" containing the normalized projections on eigenvectors
- **eVal**: Object of class "matrix" containing the corresponding eigenvalues
- **eVec**: Object of class "matrix" containing the corresponding eigenvectors
- **label**: Object of class "matrix" containing the categorical variables that the categorical data be assigned to one of the categories

Methods

- **prj** signature(object = "qkgda"): returns the normalized projections
- **eVal** signature(object = "qkgda"): returns the eigenvalues
- **eVec** signature(object = "qkgda"): returns the eigenvectors
- **kcall** signature(object = "qkgda"): returns the performed call
- **cndkernf** signature(object = "qkgda"): returns the used kernel function
- **predict** signature(object = "qkgda"): embeds new data
- **xmatrix** signature(object = "qkgda"): returns the used data matrix

Author(s)

Yusen Zhang
<yusenzhang@126.com>

See Also

- qkernel-class, cndkernel-class

Examples

```r
Iris <- data.frame(rbind(iris3[,1], iris3[,2], iris3[,3]), Sp = rep(c("1","2","3"), rep(50,3)))
testset <- sample(1:150,20)
train <- as.matrix(iris[-testset,-5])
test <- as.matrix(iris[testset,-5])
Sp = rep(c("1","2","3"), rep(50,3))
labels <-as.numeric(Sp)
trainlabel <- labels[-testset]
testlabel <- labels[testset]

kgda1 <- qkgda(train, label=trainlabel, kernel = "ratibase", qpar = list(c=1,q=0.9),features = 2)

prj(kgda1)
eVal(kgda1)
eVec(kgda1)
cndkernf(kgda1)
kcall(kgda1)
```
## qkIsomap

**qKernel Isometric Feature Mapping**

### Description

Computes the Isomap embedding as introduced in 2000 by Tenenbaum, de Silva and Langford.

### Usage

```r
## S4 method for signature 'matrix'
qkIsomap(x, kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
dims = 2, k, mod = FALSE, plotResiduals = FALSE, verbose = TRUE, na.action = na.omit, ...)
```

```r
## S4 method for signature 'cndkernmatrix'
qkIsomap(x, dims = 2, k, mod = FALSE, plotResiduals = FALSE,
verbose = TRUE, na.action = na.omit, ...)
```

```r
## S4 method for signature 'qkernmatrix'
qkIsomap(x, dims = 2, k, mod = FALSE, plotResiduals = FALSE,
verbose = TRUE, na.action = na.omit, ...)
```

### Arguments

- **x**
  
  N x D matrix (N samples, D features) or a kernel matrix of `cndkernmatrix` or `qkernmatrix`.

- **kernel**
  
  the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. qkerntool provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:
  
  - rbfbase Radial Basis qkernel function "Gaussian"
  - nonlbase Non Linear qkernel function
  - laplbase Laplbase qkernel function
  - ratibase Rational Quadratic qkernel function
  - multbase Multiquadric qkernel function
  - invbase Inverse Multiquadric qkernel function
  - wavbase Wave qkernel function
  - powbase Power qkernel function
  - logbase Log qkernel function
  - caubase Cauchy qkernel function
  - chibase Chi-Square qkernel function
  - studbase Generalized T-Student qkernel function
  - nonlcnd Non Linear cndkernel function
  - polycnd Polynomial cndkernel function
  - rbfcnd Radial Basis cndkernel function "Gaussian"
- laplcnd Laplacian cndkernel function
- anocnd ANOVA cndkernel function
- raticnd Rational Quadratic cndkernel function
- multcnd Multiquadric cndkernel function
- invcnd Inverse Multiquadric cndkernel function
- wavcnd Wave cndkernel function
- powcnd Power cndkernel function
- logcnd Log cndkernel function
- caucnd Cauchy cndkernel function
- chicnd Chi-Square cndkernel function
- studcnd Generalized T-Student cndkernel function

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

qpar

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, q for the Radial Basis qkernel function "rbfbase" , the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
- alpha, q for the Non Linear qkernel function "nonlbase".
- c, q for the Rational Quadratic qkernel function "ratibase" , the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
- theta, q for the Wave qkernel function "wavbase".
- d, q for the Power qkernel function "powbase" , the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
- alpha for the Non Linear cndkernel function "noncnd".
- d, alpha, c for the Polynomial cndkernel function "polycnd".
- gamma for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
- d, sigma for the ANOVA cndkernel function "anocnd".
- c for the Rational Quadratic cndkernel function "raticnd" , the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
- theta for the Wave cndkernel function "wavcnd".
- d for the Power cndkernel function "powcnd" , the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

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

dims vector containing the target space dimension(s)

k number of neighbours

mod use modified Isomap algorithm

plotResiduals show a plot with the residuals between the high and the low dimensional data

verbose show a summary of the embedding procedure at the end
qkIsomap

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 qkIsomap is a nonlinear dimension reduction technique, that preserves global properties of the data. That means, that geodesic distances between all samples are captured best in the low dimensional embedding.

This R version is based on the Matlab implementation by Tenenbaum and uses Floyd's Algorithm to compute the neighbourhood graph of shortest distances, when calculating the geodesic distances. A modified version of the original Isomap algorithm is included. It respects nearest and farthest neighbours.

To estimate the intrinsic dimension of the data, the function can plot the residuals between the high and the low dimensional data for a given range of dimensions.

Value

qkIsomap gives out an S4 object which is a LIST with components

- prj a N x dim matrix (N samples, dim features) with the reduced input data (list of several matrices if more than one dimension was specified).
- dims the dimension of the target space.
- Residuals the residual variances for all dimensions.
- eVal the corresponding eigenvalues.
- eVec the corresponding eigenvectors.
- cndkernf the kernel function used.
- kcall The formula of the function called

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

Author(s)

Yusen Zhang
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References

Examples

```r
# another example using the iris
data(iris)
testset <- sample(1:150,20)
train <- as.matrix(iris[-testset,-5])
labeltrain <- as.integer(iris[-testset,5])
test <- as.matrix(iris[testset,-5])
# ratibase(c=1,q=0.8)
d_low = qkIsomap(train, kernel = "ratibase", qpar = list(c=1,q=0.8),
dims=2, k=5, plotResiduals = TRUE)
# plot the data projection on the components
plot(prj(d_low),col=labeltrain, xlab="1st Principal Component",ylab="2nd Principal Component")
prj(d_low)
dims(d_low)
Residuals(d_low)
eVal(d_low)
eVec(d_low)
kcall(d_low)
cndkernf(d_low)
```

---

**qkIsomap-class**

**qKernel Isomap embedding**

**Description**

The qKernel Isometric Feature Mapping class

**Objects of class "qkIsomap"**

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

**Slots**

- `prj`: Object of class "matrix" containing the Nxdim matrix (N samples, dim features) with the reduced input data (list of several matrices if more than one dimension specified)
- `dims`: Object of class "numeric" containing the dimension of the target space (default 2)
- `connum`: Object of class "numeric" containing the number of connected components in graph
- `Residuals`: Object of class "vector" containing the residual variances for all dimensions
- `eVal`: Object of class "vector" containing the corresponding eigenvalues
- `eVec`: Object of class "vector" containing the corresponding eigenvectors
Methods

prj signature(object = "qkIsomap"): returns the Nxdim matrix (N samples, dim features)
dims signature(object = "qkIsomap"): returns the dimension
Residuals signature(object = "qkIsomap"): returns the residual variances
eVal signature(object = "qkIsomap"): returns the eigenvalues
eVec signature(object = "qkIsomap"): returns the eigenvectors
xmatrix signature(object = "qkIsomap"): returns the used data matrix
kcall signature(object = "qkIsomap"): returns the performed call
cndkernf signature(object = "qkIsomap") : returns the used kernel function

Author(s)

Yusen Zhang
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See Also

qkernel-class, cndkernel-class, qkIsomap

Examples

# another example using the iris data
data(iris)
testset <- sample(1:150,20)
train <- as.matrix(iris[-testset,-5])
labeltrain <- as.integer(iris[-testset,5])
test <- as.matrix(iris[testset,-5])
# ratibase(c=1, q=0.8)
d_low = qkIsomap(train, kernel = "ratibase", qpar = list(c=1, q=0.8),
                dims=2, k=5, plotResiduals = TRUE)
# plot the data projection on the components
plot(prj(d_low), col=labeltrain, xlab="1st Principal Component", ylab="2nd Principal Component")

prj(d_low)
dims(d_low)
Residuals(d_low)
eVal(d_low)
eVec(d_low)
kcall(d_low)
cndkernf(d_low)
qkLLE

qKernel Locally Linear Embedding

Description

Computes the qkernel Locally Linear Embedding

Usage

## S4 method for signature 'matrix'
qkLLE(x, kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
   dims = 2, k, na.action = na.omit, ...)
## S4 method for signature 'cndkernmatrix'
qkLLE(x, dims = 2, k, na.action = na.omit, ...)
## S4 method for signature 'qkernmatrix'
qkLLE(x, dims = 2, k, na.action = na.omit,...)

Arguments

x             N x D matrix (N samples, D features) or a kernel matrix of cndkernmatrix or qkernmatrix.
kernel        the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. qkerntool provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:
   • rbfbase Radial Basis qkernel function "Gaussian"
   • nonlbase Non Linear qkernel function
   • laplbase Laplbase qkernel function
   • ratibase Rational Quadratic qkernel function
   • multbase Multiquadric qkernel function
   • invbbase Inverse Multiquadric qkernel function
   • wavbase Wave qkernel function
   • powbase Power qkernel function
   • logbbase Log qkernel function
   • caubase Cauchy qkernel function
   • chibase Chi-Square qkernel function
   • studbase Generalized T-Student qkernel function
   • nonlcnd Non Linear cndkernel function
   • polycnd Polynomial cndkernel function
   • rbfncnd Radial Basis cndkernel function "Gaussian"
   • laplcnd Laplacian cndkernel function
   • anocnd ANOVA cndkernel function
   • raticnd Rational Quadratic cndkernel function
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:

- \( \sigma, q \) for the Radial Basis kernel function "rbfbase", the Laplacian kernel function "laplbase" and the Cauchy kernel function "caubase".
- \( \alpha, q \) for the Non Linear kernel function "nonlbase".
- \( \gamma, q \) for the Rational Quadratic kernel function "ratibase", the Multiquadric kernel function "multbase" and the Inverse Multiquadric kernel function "invbase".
- \( \theta, q \) for the Wave kernel function "wavbase".
- \( d, q \) for the Power kernel function "powbase", the Log kernel function "logbase" and the Generalized T-Student kernel function "studbase".
- \( \alpha \) for the Non Linear cndkernel function "nonlcnd".
- \( \text{power}, \alpha, c \) for the Polynomial cndkernel function "polycnd".
- \( \gamma \) for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
- \( \text{power}, \sigma \) for the ANOVA cndkernel function "anocnd".
- \( c \) for the Rational Quadratic cndkernel function "raticnd", the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
- \( \theta \) for the Wave cndkernel function "wavcnd".
- \( \text{power} \) for the Power cndkernel function "powcnd", the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

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

dims dimension of the target space

k the number of nearest neighbours.

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.)

\( \ldots \) additional parameters
Details

The qkernel Locally Linear Embedding (qkLLE) preserves local properties of the data by representing each sample in the data by a linear combination of its k nearest neighbours with each neighbour weighted independently. qkLLE finally chooses the low-dimensional representation that best preserves the weights in the target space. It is an extension of Locally Linear Embedding (LLE) with qkernel method.

Value

It returns an S4 object containing the principal component vectors along with the corresponding eigenvalues.

- `prj`: a matrix with the reduced input data
- `dims`: dimension of the target space
- `eVal`: The corresponding eigenvalues
- `eVec`: The corresponding eigenvectors
- `cndkernf`: the kernel function used

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

Author(s)

Yusen Zhang
<yusenzhang@126.com>

References

Roweis, Sam T. and Saul, Lawrence K., "Nonlinear Dimensionality Reduction by Locally Linear Embedding", 2000;

Examples

```r
## S4 method for signature 'matrix'
data(iris)
testset <- sample(1:150, 20)
train <- as.matrix(iris[-testset,-5])
labeltrain<- as.integer(iris[-testset,5])
test <- as.matrix(iris[testset,-5])
plot(train ,col=labeltrain, xlab="1st Principal Component",ylab="2nd Principal Component")
# ratibase(c=1,q=0.8)
d_low <- qkLLE(train, kernel = "ratibase", qpar = list(c=1,q=0.8), dims=2, k=5)
# plot the data projection on the components
plot(prj(d_low),col=labeltrain, xlab="1st Principal Component",ylab="2nd Principal Component")

## S4 method for signature 'qkernmatrix'
# ratibase(c=0.1,q=0.8)
qkfunc <- ratibase(c=0.1,q=0.8)
ktrainl <- qkernmatrix(qkfunc,train)
d_low <- qkLLE(ktrainl, dims = 2, k=5)
```
# plot the data projection on the components
plot(prj(d_low), col=labeltrain, xlab="1st Principal Component", ylab="2nd Principal Component")

## qkLLE-class

### Description

The qKernel Locally Linear Embedding class

### Objects of class "qkLLE"

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

### Slots

- **prj**: Object of class "matrix" containing the reduced input data
- **dims**: Object of class "numeric" containing the dimension of the target space (default 2)
- **eVal**: Object of class "vector" containing the corresponding eigenvalues
- **eVec**: Object of class "matrix" containing the corresponding eigenvectors

### Methods

- **prj** signature(object = "qkLLE"): returns the reduced input data
- **dims** signature(object = "qkLLE"): returns the dimension
- **eVal** signature(object = "qkLLE"): returns the eigenvalues
- **eVec** signature(object = "qkLLE"): returns the eigenvectors
- **xmatrix** signature(object = "qkLLE"): returns the used data matrix
- **kcall** signature(object = "qkLLE"): returns the performed call
- **cndkernf** signature(object = "qkLLE"): returns the used kernel function

### Author(s)

Yusen Zhang
<yusenzhang@126.com>

### See Also

qkernel-class, cndkernel-class
Examples

```r
## S4 method for signature 'matrix'
data(iris)
testset <- sample(1:150, 20)
train <- as.matrix(iris[-testset,-5])
labeltrain <- as.integer(iris[-testset,5])
test <- as.matrix(iris[testset,-5])
plot(train, col=labeltrain, xlab="1st Principal Component", ylab="2nd Principal Component")
# ratibase(c=1,q=0.8)
d_low <- qkLLE(train, kernel = "ratibase", qpar = list(c=1,q=0.8), dims=2, k=5)
# plot the data projection on the components
plot(prj(d_low), col=labeltrain, xlab="1st Principal Component", ylab="2nd Principal Component")

## S4 method for signature 'qkernmatrix'
# ratibase(c=0.1,q=0.8)
qkfunc <- ratibase(c=0.1,q=0.8)
ktrain1 <- qkernmatrix(qkfunc, train)
d_low <- qkLLE(ktrain1, dims=2, k=5)
# plot the data projection on the components
plot(prj(d_low), col=labeltrain, xlab="1st Principal Component", ylab="2nd Principal Component")
```

qkMDS

qKernel Metric Multi-Dimensional Scaling

Description

The qkernel Metric Multi-Dimensional Scaling is a nonlinear form of Metric Multi-Dimensional Scaling

Usage

```r
## S4 method for signature 'matrix'
qkMDS(x, kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
dims = 2, plotResiduals = FALSE, verbose = TRUE, na.action = na.omit, ...)

## S4 method for signature 'cndkernmatrix'
qkMDS(x, dims = 2, plotResiduals = FALSE,
verbose = TRUE, na.action = na.omit, ...)

## S4 method for signature 'qkernmatrix'
qkMDS(x, dims = 2, plotResiduals = FALSE,
verbose = TRUE, na.action = na.omit, ...)
```

Arguments

- `x`: N x D matrix (N samples, D features) or a kernel matrix of cndkernmatrix or qkernmatrix.
the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. qkerntool provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:

- rbfbase Radial Basis qkernel function "Gaussian"
- nonlbase Non Linear qkernel function
- laplbase Laplbase qkernel function
- ratibase Rational Quadratic qkernel function
- multbase Multiquadric qkernel function
- invbase Inverse Multiquadric qkernel function
- wavbase Wave qkernel function
- powbase Power qkernel function
- logbase Log qkernel function
- caubase Cauchy qkernel function
- chibase Chi-Square qkernel function
- studbase Generalized T-Student qkernel function
- nonlcnd Non Linear cnndkernel function
- polycnd Polynomial cnndkernel function
- rbfcnnd Radial Basis cnndkernel function "Gaussian"
- laplcnnd Laplacian cnndkernel function
- anocnd ANOVA cnndkernel function
- raticnd Rational Quadratic cnndkernel function
- multcnnd Multiquadric cnndkernel function
- invcnnd Inverse Multiquadric cnndkernel function
- wavcnnd Wave cnndkernel function
- powcnnd Power cnndkernel function
- logcnnd Log cnndkernel function
- caucnnd Cauchy cnndkernel function
- chicnnd Chi-Square cnndkernel function
- studcnnd Generalized T-Student cnndkernel function

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, q for the Radial Basis qkernel function "rbfbase", the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
- alpha, q for the Non Linear qkernel function "nonlbase".
- c, q for the Rational Quadratic qkernel function "ratibase", the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
- theta, q for the Wave qkernel function "wavbase".
- \( d, q \) for the Power qkernel function "powbase", the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
- \( \alpha \) for the Non Linear cndkernel function "noncnd".
- \( d, \alpha, c \) for the Polynomial cndkernel function "polycnd".
- \( \gamma \) for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
- \( d, \sigma \) for the ANOVA cndkernel function "anocnd".
- \( c \) for the Rational Quadratic cndkernel function "raticnd", the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
- \( \theta \) for the Wave cndkernel function "wavcnd".
- \( d \) for the Power cndkernel function "powcnd", the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

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

- `dims` vector containing the target space dimension(s)
- `plotResiduals` show a plot with the residuals between the high and the low dimensional data
- `verbose` show a summary of the embedding procedure at the end
- `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**

There are several versions of non-metric multidimensional scaling in R, but `qkerntool` offers the following unique combination of using qKernel methods

**Value**

`qkMDS` gives out an S4 object which is a LIST with components

- `prj` a N x dim matrix (N samples, dim features) with the reduced input data (list of several matrices if more than one dimension was specified).
- `dims` the dimension of the target space.
- `Residuals` the residual variances for all dimensions.
- `eVal` the corresponding eigenvalues.
- `eVec` the corresponding eigenvectors.
- `cndkernf` the kernel function used.
- `kcall` The formula of the function called

all the slots of the object can be accessed by accessor functions.
Author(s)

Yusen Zhang
<yusenzhang@126.com>

References


Examples

```r
# another example using the iris
data(iris)
testset <- sample(1:150, 20)
train <- as.matrix(iris[-testset,-5])
labeltrain <- as.integer(iris[-testset,5])
test <- as.matrix(iris[testset,-5])

# ratibase(c=1,q=0.8)
d_low = qkMDS(train, kernel = "ratibase", qpar = list(c=1,q=0.9), dims = 2, plotResiduals = TRUE)

# plot the data projection on the components
plot(prj(d_low), col=labeltrain, xlab="1st Principal Component", ylab="2nd Principal Component")

prj(d_low)
dims(d_low)
Residuals(d_low)
eVal(d_low)
eVec(d_low)
kcall(d_low)
cndkernf(d_low)
```

qkMDS-class

**qKernel Metric Multi-Dimensional Scaling**

Description

The qkernel Metric Multi-Dimensional Scaling class

Objects of class "qkMDS"

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

Slots

- `prj`: Object of class "matrix" containing the Nxdim matrix (N samples, dim features) with the reduced input data (list of several matrices if more than one dimension specified)
- `dims`: Object of class "numeric" containing the dimension of the target space (default 2)
- `connum`: Object of class "numeric" containing the number of connected components in graph
Residuals: Object of class "vector" containing the residual variances for all dimensions

eVal: Object of class "vector" containing the corresponding eigenvalues

eVec: Object of class "vector" containing the corresponding eigenvectors

Methods

prj signature(object = "qkMDS"): returns the Nxdim matrix (N samples, dim features)

dims signature(object = "qkMDS"): returns the dimension

Residuals signature(object = "qkMDS"): returns the residual variances

eVal signature(object = "qkMDS"): returns the eigenvalues

eVec signature(object = "qkMDS"): returns the eigenvectors

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

kcall signature(object = "qkMDS"): returns the performed call

cndkernf signature(object = "qkMDS"): returns the used kernel function

Author(s)

Yusen Zhang
<yusenzhang@126.com>

See Also

qkernel-class, cndkernel-class, qkMDS

Examples

# another example using the iris
data(iris)
testset <- sample(1:150,20)
train <- as.matrix(iris[-testset,-5])
labeltrain<- as.integer(iris[-testset,5])
test <- as.matrix(iris[testset,-5])

# ratibase(c=1,q=0.8)
d_low = qkMDS(train, kernel = "ratibase", qpar = list(c=1,q=0.8),
dims=2, plotResiduals = TRUE)

# plot the data projection on the components
plot(prj(d_low),col=labeltrain, xlab="1st Principal Component",ylab="2nd Principal Component")

prj(d_low)
dims(d_low)
Residuals(d_low)
eVal(d_low)
eVec(d_low)
kcall(d_low)
cndkernf(d_low)
qkpca

qKernel Principal Components Analysis

Description
The qkernel Principal Components Analysis is a nonlinear form of principal component analysis.

Usage

```r
## S4 method for signature 'formula'
qkpca(x, data = NULL, na.action, ...)
## S4 method for signature 'matrix'
qkpca(x, kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
       features = 0, th = 1e-4, na.action = na.omit, ...)
## S4 method for signature 'cndkernmatrix'
qkpca(x, features = 0, th = 1e-4, ...)
## S4 method for signature 'qkernmatrix'
qkpca(x, features = 0, th = 1e-4, ...)
```

Arguments

- **x** the data matrix indexed by row, a formula describing the model or a kernel matrix of `cndkernmatrix` or `qkernmatrix`.
- **data** an optional data frame containing the variables in the model (when using a formula).
- **kernel** the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. `qkerntool` provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:
  - `rbfbase` Radial Basis qkernel function "Gaussian"
  - `nonlbase` Non Linear qkernel function
  - `laplbase` Laplbase qkernel function
  - `ratibase` Rational Quadratic qkernel function
  - `multbase` Multiquadric qkernel function
  - `invbase` Inverse Multiquadric qkernel function
  - `wavbase` Wave qkernel function
  - `powbase` d qkernel function
  - `logbase` Log qkernel function
  - `caubase` Cauchy qkernel function
  - `chibase` Chi-Square qkernel function
  - `studbase` Generalized T-Student qkernel function
  - `nonlcnd` Non Linear cndkernel function
  - `polycnd` Polynomial cndkernel function
  - `rbfcnd` Radial Basis cndkernel function "Gaussian"
qpar

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

qpar

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, q for the Radial Basis qkernel function "rbfbase", the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
- alpha, q for the Non Linear qkernel function "nonlbase".
- c, q for the Rational Quadratic qkernel function "ratibase", the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
- theta, q for the Wave qkernel function "wavbase".
- d, q for the d qkernel function "powbase", the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
- alpha for the Non Linear cndkernel function "nonlcnd".
- d, alpha, c for the Polynomial cndkernel function "polycnd".
- gamma for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
- d, sigma for the ANOVA cndkernel function "anocnd".
- c for the Rational Quadratic cndkernel function "raticnd", the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
- theta for the Wave cndkernel function "wavcnd".
- d for the power cndkernel function "powcnd", the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

Hyper-parameters for user defined kernels can be passed through the qpar 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.)
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 \texttt{qkpca} function in a matrix, in addition \texttt{qkpca} also supports input in the form of a kernel matrix of class \texttt{qkernmatrix} or class \texttt{cndkernmatrix}.

Value

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

- \texttt{pcv} a matrix containing the principal component vectors (column wise)
- \texttt{eVal} The corresponding eigenvalues
- \texttt{rotated} The original data projected (rotated) on the principal components
- \texttt{cndkernf} the kernel function used
- \texttt{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)

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References

Schoelkopf B., A. Smola, K.-R. Mueller:

*Nonlinear component analysis as a kernel eigenvalue problem*

Neural Computation 10, 1299-1319

http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.29.1366

See Also

- \texttt{qkernmatrix}, \texttt{cndkernmatrix}

Examples

```r
# another example using the iris data
data(iris)
test <- sample(1:150,20)
qkpc <- qkpca(~.,data=iris[-test,-5],kernel="rbfbase",
             qpar=list(sigma=50,q=0.8),features=2)

# print the principal component vectors
```
qkpca-class

Description

The qkernel Principal Components Analysis class

Objects of class "qkpca"

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

Slots

- **pcv**: Object of class "matrix" containing the principal component vectors
- **eVal**: Object of class "vector" containing the corresponding eigenvalues
- **rotated**: Object of class "matrix" containing the projection of the data on the principal components

Methods

- **eVal** signature(object = "qkpca"): returns the eigenvalues
- **pcv** signature(object = "qkpca"): returns the principal component vectors
- **predict** signature(object = "qkpca"): embeds new data
- **rotated** signature(object = "qkpca"): returns the projected data
- **xmatrix** signature(object = "qkpca"): returns the used data matrix
- **kcarnf** signature(object = "qkpca"): returns the performed call
- **cndkernelf** signature(object = "qkpca"): returns the used kernel function

Author(s)

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See Also

qkernel-class, cndkernel-class
Examples

# another example using the iris data
data(iris)
test <- sample(1:150,20)
qkpc <- qkpca(~.,iris[-test,-5], kernel = "rbfbase",
            qpar = list(sigma = 50, q = 0.8), features = 2)

# print the principal component vectors
pcv(qkpc)
rotated(qkpc)
cndkernf(qkpc)
eVal(qkpc)
xmatrix(qkpc)
names(eVal(qkpc))

---

qkprc-class  Class "qkprc"

Description

The qKernel Prehead class

Objects of class "qkprc"

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

Slots

cndkernf: Object of class "kfunction" containing the kernel function used
qpar: Object of class "list" containing the kernel parameters used
xmatrix: Object of class "input" containing the data matrix used
ymatrix: Object of class "input" containing the data matrix used
kcall: Object of class "ANY" containing the function call
terms: Object of class "ANY" containing the function terms
n.action: Object of class "ANY" containing the action performed on NA

Methods

cndkernf  signature(object = "qkprc"): returns the used kernel function
xmatrix  signature(object = "qkprc"): returns the used data matrix
ymatrix  signature(object = "qkprc"): returns the used data matrix
kcall  signature(object = "qkprc"): returns the performed call

Author(s)

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See Also
qkernel-class, cndkernel-class

qkspecc  
qkernel spectral Clustering

Description
A qkernel spectral clustering algorithm. Clustering is performed by embedding the data into the subspace of the eigenvectors of a graph Laplacian matrix.

Usage
```r
## S4 method for signature 'matrix'
qkspecc(x, kernel = "rbfbase", qpar = list(sigma = 2, q = 0.9),
        Nocent = NA, normalize = "symmetric", maxk = 20, iterations = 200,
        na.action = na.omit, ...)

## S4 method for signature 'cndkernmatrix'
qkspecc(x, Nocent = NA, normalize = "symmetric",
        maxk = 20, iterations = 200, ...)

## S4 method for signature 'qkernmatrix'
qkspecc(x, Nocent = NA, normalize = "symmetric",
        maxk = 20, iterations = 200, ...)
```

Arguments
- `x`  
  the matrix of data to be clustered or a kernel Matrix of class qkernmatrix or cndkernmatrix.
- `kernel`  
  the kernel function used in computing the affinity matrix. This parameter can be set to any function, of class kernel, which computes a kernel function value between two vector arguments. kernlab provides the most popular kernel functions which can be used by setting the kernel parameter to the following strings:
  - `rbfbase`  Radial Basis qkernel function "Gaussian"
  - `nonlbase`  Non Linear qkernel function
  - `laplbase`  Laplbase qkernel function
  - `ratibase`  Rational Quadratic qkernel function
  - `multbase`  Multiquadric qkernel function
  - `invbase`  Inverse Multiquadric qkernel function
  - `wavbase`  Wave qkernel function
  - `powbase`  d qkernel function
  - `logbase`  Log qkernel function
  - `caubase`  Cauchy qkernel function
• chi.base Chi-Square qkernel function
• stud.base Generalized T-Student qkernel function
• nonlcnd Non Linear cndkernel function
• polyclnd Polynomial cndkernel function
• rbfclnd Radial Basis cndkernel function "Gaussian"
• laplclnd Laplacian cndkernel function
• anocnd ANOVA cndkernel function
• raticclnd Rational Quadratic cndkernel function
• multclnd Multiquadric cndkernel function
• invclnd Inverse Multiquadric cndkernel function
• wavclnd Wave cndkernel function
• powclnd d cndkernel function
• logclnd Log cndkernel function
• caucnd Cauchy cndkernel function
• chicnd Chi-Square cndkernel function
• studclnd Generalized T-Student cndkernel function

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

qpar

a character string or the list of hyper-parameters (kernel parameters). The default character string list(sigma = 2, q = 0.9) 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 multiple scales. A list can also be used containing the parameters to be used with the kernel function. Valid parameters for existing kernels are:

• sigma, q for the Radial Basis qkernel function "rbfbase", the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
• alpha, q for the Non Linear qkernel function "nonlbase".
• c, q for the Rational Quadratic qkernel function "ratibase", the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
• theta, q for the Wave qkernel function "wavbase".
• d, q for the d qkernel function "powbase", the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
• alpha for the Non Linear cndkernel function "nonlcnd".
• d, alpha, c for the Polynomial cndkernel function "polyclnd".
• gamma for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
• d, sigma for the ANOVA cndkernel function "anocnd".
• c for the Rational Quadratic cndkernel function "raticclnd", the Multiquadric cndkernel function "multclnd" and the Inverse Multiquadric cndkernel function "invclnd".
• theta for the Wave cndkernel function "wavclnd".
• d for the d cndkernel function "powcnd", the Log cndkernel function "logcnd"
and the Generalized T-Student cndkernel function "studcnd". where length
is the length of the strings considered, lambda the decay factor and nor-
malized a logical parameter determining if the kernel evaluations should be
normalized.

Hyper-parameters for user defined kernels can be passed through the qpar pa-
rameter as well.

Nocent the number of clusters.
normalize Normalisation of the Laplacian ("none", "symmetric" or "random-walk").
maxk If k is NA, an upper bound for the automatic estimation. Defaults to 20.
iterations the maximum number of iterations allowed.
na.action the action to perform on NA.
... additional parameters.

Details

The qkernel spectral clustering works by embedding the data points of the partitioning problem into
the subspace of the eigenvectors corresponding to the \( k \) smallest eigenvalues of the graph Laplacian
matrix. Using a simple clustering method like kmeans on the embedded points usually leads to
good performance. It can be shown that qkernel spectral clustering methods boil down to graph
partitioning.

The data can be passed to the qkspecc function in a matrix, in addition qkspecc also supports
input in the form of a kernel matrix of class qkernmatrix or cndkernmatrix.

Value

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

clust The cluster assignments
eVec The corresponding eigenvector
eVal The corresponding eigenvalues
ymatrix The eigenvectors corresponding to the \( k \) smallest eigenvalues of the graph Lapla-
cian matrix.

Author(s)

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References

Andrew Y. Ng, Michael I. Jordan, Yair Weiss
On Spectral Clustering: Analysis and an Algorithm
Neural Information Processing Symposium 2001
qkspecc-class

See Also
qkernmatrix, cndkernmatrix, qkpc

Examples

data("iris")
x=as.matrix(iris[,,-5])

qspe <- qkspecc(x,kernel = "rbfbase", qpar = list(sigma = 10, q = 0.9),
       Nocent=3, normalize="symmetric", maxk=15, iterations=1200)
plot(x, col = clust(qspe))

qkfunc <- nonlbase(alpha=1/15,q=0.8)
Ktrain <- qkernmatrix(qkfunc, x)
qspe <- qkspecc(Ktrain, Nocent=3, normalize="symmetric", maxk=20)
plot(x, col = clust(qspe))

qkspecc-class

Class “qkspecc”

Description
The qKernel Spectral Clustering Class

Objects from the Class

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

Slots
clust: Object of class "vector" containing the cluster assignments
eVec: Object of class "matrix" containing the corresponding eigenvector in each cluster
eVal: Object of class "vector" containing the corresponding eigenvalue for each cluster
withinss: Object of class "vector" containing the within-cluster sum of squares for each cluster

Methods
clust signature(object = "qkspecc"): returns the cluster assignments
eVec signature(object = "qkspecc"): returns the corresponding eigenvector in each cluster
eVal signature(object = "qkspecc"): returns the corresponding eigenvalue for each cluster
xmatrix signature(object = "qkspecc"): returns the original data matrix or a kernel Matrix
ymatrix signature(object = "qkspecc"): returns The eigenvectors corresponding to the k smallest eigenvalues of the graph Laplacian matrix.
cndkernf signature(object = "qkspecc"): returns the used kernel function
kcall signature(object = "qkspecc"): returns the performed call
Author(s)
Yusen Zhang
<yusenzhang@126.com>

See Also
qkspecc, qkernel-class, cndkernel-class

Examples
## Cluster the iris data set.
data("iris")
x=as.matrix(iris[, -5])
qspe <- qkspecc(x, kernel = "rbfbase", qpar = list(sigma = 10, q = 0.9),
               Nocent = 3, normalize = "symmetric", maxk = 15, iterations = 1200)
clust(qspe)
eVec(qspe)
eVal(qspe)
xmatrix(qspe)
ymatrix(qspe)
cndkernf(qspe)

qkspeclust  qkernel spectral Clustering

Description
This is also a qkernel spectral clustering algorithm which uses three ways to assign labels after the laplacian embedding: kmeans, hclust and dbscan.

Usage
## S4 method for signature 'qkspecc'
qkspeclust(x, clustmethod = "kmeans",
           Nocent = NULL, iterations = NULL, hmethod = NULL, eps = NULL, MinPts = NULL)

Arguments
  x               object of class qkspecc.
  clustmethod    the strategy to use to assign labels in the embedding space. There are three ways to assign labels after the laplacian embedding: kmeans, hclust and dbscan.
  Nocent         the number of clusters
  iterations     the maximum number of iterations allowed for "kmeans".
  hmethod        the agglomeration method for "hclust". This should be (an unambiguous abbreviation of) one of "ward.D", "ward.D2", "single", "complete", "average" (= UPGMA), "mcquitty" (= WPGMA), "median" (= WPGMC) or "centroid" (= UPGMC).
eps  Reachability distance for "dbscan".
MinPts  Reachability minimum no. of points for "dbscan".

Details

The qkernel spectral clustering works by embedding the data points of the partitioning problem into the subspace of the eigenvectors corresponding to the $k$ smallest eigenvalues of the graph Laplacian matrix. Using the simple clustering methods like kmeans, hclust and dbscan on the embedded points usually leads to good performance. It can be shown that qkernel spectral clustering methods boil down to graph partitioning.

Value

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

- clust  The cluster assignments
- eVec  The corresponding eigenvector
- eVal  The corresponding eigenvalues
- xmatrix  The original data matrix
- ymatrix  The real valued matrix of eigenvectors corresponding to the $k$ smallest eigenvalues of the graph Laplacian matrix
- cndkernf  The kernel function used

Author(s)

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References

Andrew Y. Ng, Michael I. Jordan, Yair Weiss
On Spectral Clustering: Analysis and an Algorithm
Neural Information Processing Symposium 2001

See Also

qkernmatrix, cndkernmatrix, qkspecc-class, qkspecc

Examples

data("iris")
x=as.matrix(iris[,,-5])

qspe <- qkspecc(x,kernel = "rbfbase", qpar = list(sigma = 90, q = 0.9),
                 Nocent=3, normalize="symmetric", maxk=15,iterations=1200)
plot(x, col = clust(qspe))
qsammon <- qkspeclust(qspe, clustmethod = "hclust", Nocent=3, hmethod="ward.D2")
plot(x, col = clust(qspec))
plot(qspec)

qKernel Sammon Mapping

Description

The qkernel Sammon Mapping is an implementation for Sammon mapping, one of the earliest
dimension reduction techniques that aims to find low-dimensional embedding that preserves pair-
wise distance structure in high-dimensional data space. qsammon is a nonlinear form of Sammon
Mapping.

Usage

## S4 method for signature 'matrix'
qsammon(x, kernel = "rbfbase", qpar = list(sigma = 0.5, q = 0.9),
dims = 2, Initialisation = 'random', MaxHalves = 20,
MaxIter = 500, TolFun = 1e-7, na.action = na.omit, ...)

## S4 method for signature 'cndkernmatrix'
qsammon(cndkernel, x, k, dims = 2, Initialisation = 'random',
MaxHalves = 20, MaxIter = 500, TolFun = 1e-7, ...)

## S4 method for signature 'qkernmatrix'
qsammon(qkernel, x, k, dims = 2, Initialisation = 'random',
MaxHalves = 20, MaxIter = 500, TolFun = 1e-7, ...)

Arguments

x

the data matrix indexed by row or a kernel matrix of cndkernmatrix or qkernmatrix.

kernel

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

- rbfbase Radial Basis qkernel function "Gaussian"
- nonlbase Non Linear qkernel function
- laplbase Laplace qkernel function
- ratibase Rational Quadratic qkernel function
- multibase Multiquadric qkernel function
- invbase Inverse Multiquadric qkernel function
- wavbase Wave qkernel function
- powbase d qkernel function
- logbase Log qkernel function
- caubase Cauchy qkernel function
- chibase Chi-Square qkernel function
- studbase Generalized T-Student qkernel function
- nonlcnd Non Linear cndkernel function
- polycnd Polynomial cndkernel function
- rbfced Radial Basis cndkernel function "Gaussian"
- laplcnd Laplacian cndkernel function
- anocnd ANOVA cndkernel function
- raticnd Rational Quadratic cndkernel function
- multcnd Multiquadric cndkernel function
- invcnd Inverse Multiquadric cndkernel function
- wavcnd Wave cndkernel function
- powcnd d cndkernel function
- logcnd Log cndkernel function
- caucnd Cauchy cndkernel function
- chicnd Chi-Square cndkernel function
- studcnd Generalized T-Student cndkernel function

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

qpar

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, q for the Radial Basis qkernel function "rbfbase" , the Laplacian qkernel function "laplbase" and the Cauchy qkernel function "caubase".
- alpha, q for the Non Linear qkernel function "nonlbase".
- c, q for the Rational Quadratic qkernel function "ratibase" , the Multiquadric qkernel function "multbase" and the Inverse Multiquadric qkernel function "invbase".
- theta, q for the Wave qkernel function "wavbase".
- d, q for the d qkernel function "powbase" , the Log qkernel function "logbase" and the Generalized T-Student qkernel function "studbase".
- alpha for the Non Linear cndkernel function "nonlcnd".
- d, alpha, c for the Polynomial cndkernel function "polycnd".
- gamma for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".
- d, sigma for the ANOVA cndkernel function "anocnd".
- c for the Rational Quadratic cndkernel function "raticnd" , the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
- theta for the Wave cndkernel function "wavcnd".
qsammon

- d for the d cndkernel function "powcnd", the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

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

qkernel the kernel function to be used to calculate the qkernel matrix.
cndkernel the cndkernel function to be used to calculate the CND kernel matrix.
k the dimension of the original data.
dims Number of features to return. (default: 2)

Initialisation "random" or "pca": the former performs fast random projection and the latter performs standard PCA (default: "random")

MaxHalves maximum number of step halvings. (default: 20)
MaxIter the maximum number of iterations allowed. (default: 500)
TolFun relative tolerance on objective function. (default: 1e-7)
n.a. 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 qsammon function in a matrix, in addition qsammon also supports input in the form of a kernel matrix of class qkernmatrix or class cndkernmatrix.

Value

dimRed The matrix whose rows are embedded observations.
kcall The function call contained
cndkernf The kernel function used

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

Author(s)

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References


See Also

qkernmatrix, cndkernmatrix
Examples

data(iris)
train <- as.matrix(iris[,1:4])
labeltrain<- as.integer(iris[,5])
## S4 method for signature 'matrix'
kpc2 <- qsammon(train, kernel = "rbfbase", qpar = list(sigma = 2, q = 0.9), dims = 2,
               Initialisation = 'pca', TolFun = 1e-5)
plot(dimRed(kpc2), col = as.integer(labeltrain))
cndkernf(kpc2)

qsammon-class  

Class "qsammon"

Description

The qKernel Sammon Mapping class

Objects of class "qsammon"

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

Slots

dimRed: Object of class "matrix" containing the matrix whose rows are embedded observations
cndkernf: Object of class "function" containing the kernel function used
kcall: Object of class "ANY" containing the function call

Methods

dimRed signature(object = "qsammon"): returns the matrix whose rows are embedded observations
kcall signature(object = "qsammon"): returns the performed call
cndkernf signature(object = "qsammon"): returns the used kernel function

Author(s)

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See Also

qsammon
Examples

data(iris)
train <- as.matrix(iris[,1:4])
labeltrain<- as.integer(iris[,5])
## S4 method for signature 'matrix'
qkpc <- qsammon(train, kernel = "rbfbase", qpar = list(sigma = 0.5, q = 0.9),
dims = 2, Initialisation = 'pca', MaxHalves = 50)
cndkernf(qkpc)
dimRed(qkpc)
kcall(qkpc)

qtSNE  qKernel t-Distributed Stochastic Neighbor Embedding

Description

Wrapper for the qkernel t-distributed stochastic neighbor embedding. qtSNE is a method for
constructing a low dimensional embedding of high-dimensional data, distances or similarities.

Usage

## S4 method for signature 'matrix'
qtSNE(x,kernel = "rbfbase", qpar = list(sigma = 0.1, q = 0.9),
initial_config = NULL, no_dims=2, initial_dims=30, perplexity=30, max_iter=1300,
min_cost=0, epoch_callback=NULL, epoch=100, na.action = na.omit, ...)
## S4 method for signature 'cndkernmatrix'
qtSNE(x,initial_config = NULL, no_dims=2, initial_dims=30,
perplexity=30, max_iter = 1000, min_cost=0, epoch_callback=NULL, epoch=100)
## S4 method for signature 'qkernmatrix'
qtSNE(x,initial_config = NULL, no_dims=2, initial_dims=30,
perplexity=30, max_iter = 1000, min_cost=0, epoch_callback=NULL, epoch=100)

Arguments

x the matrix of data to be clustered or a kernel Matrix of class qkernmatrix or
   cndkernmatrix.
kernel the kernel function used in computing the affinity matrix. This parameter can be
   set to any function, of class kernel, which computes a kernel function value be-
   tween two vector arguments. kernlab provides the most popular kernel functions
   which can be used by setting the kernel parameter to the following strings:
   • rbfbase Radial Basis qkernel function "Gaussian"
   • nonlbase Non Linear qkernel function
   • laplbase Laplbase qkernel function
   • ratibase Rational Quadratic qkernel function
• multbase Multiquadric qkernel function
• invbase Inverse Multiquadric qkernel function
• wavbase Wave qkernel function
• powbase Power qkernel function
• logbase Log qkernel function
• caubase Cauchy qkernel function
• chibase Chi-Square qkernel function
• studbase Generalized T-Student qkernel function
• nonlcnd Non Linear cndkernel function
• polycnd Polynomial cndkernel function
• rbfcnd Radial Basis cndkernel function "Gaussian"
• laplncnd Laplacian cndkernel function
• anocnd ANOVA cndkernel function
• raticnd Rational Quadratic cndkernel function
• multcnd Multiquadric cndkernel function
• invcnd Inverse Multiquadric cndkernel function
• wavcnd Wave cndkernel function
• powcnd Power cndkernel function
• logcnd Log cndkernel function
• caucnd Cauchy cndkernel function
• chicnd Chi-Square cndkernel function
• studcnd Generalized T-Student cndkernel function

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

qpar

a character string or the list of hyper-parameters (kernel parameters). The default character string `list(sigma = 2, q = 0.9)` 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 multiple scales. A list can also be used containing the parameters to be used with the kernel function. Valid parameters for existing kernels are:

• sigma for the Radial Basis qkernel function "rbfbase", the Laplacian qkernel function "laplbase" the Cauchy qkernel function "caubase" and for the ANOVA cndkernel function "anocnd".
• alpha for the Non Linear qkernel function "nonlbase", for the Non Linear cndkernel function "nonlcnd", and for the Polynomial cndkernel function "polycnd".
• c for the Rational Quadratic qkernel function "ratibase", the Multiquadric qkernel function "multbase", the Inverse Multiquadric qkernel function "invbase", for the Polynomial cndkernel function "polycnd", for the Rational Quadratic cndkernel function "raticnd", the Multiquadric cndkernel function "multcnd" and the Inverse Multiquadric cndkernel function "invcnd".
• d for qkernel function "powbase", the Log qkernel function "logbase", the Generalized T-Student qkernel function "studbase", for the Polynomial cndkernel function "polycnd", for the ANOVA cndkernel function "anocnd", for the d cndkernel function "powcnd", the Log cndkernel function "logcnd" and the Generalized T-Student cndkernel function "studcnd".

• theta for the Wave qkernel function "wavbase" and for the Wave cndkernel function "wavcnd".

• gamma for the Chi-Square qkernel function "chibase", for the Radial Basis cndkernel function "rbfcnd" and the Laplacian cndkernel function "laplcnd" and the Cauchy cndkernel function "caucnd".

• q For all qkernel Function. 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 qkpar parameter as well.

initial_config An intitial configure about x (default: NULL)
no_dims the dimension of the resulting embedding. (default: 2)
initial_dims The number of dimensions to use in reduction method. (default: 30)
perplexity Perplexity parameter
max_iter Number of iterations (default: 1300)
min_cost The minimum cost for every object after the final iteration
epoch_callback A callback function used after each epoch (an epoch here means a set number of iterations)
epoch The interval of the number of iterations displayed (default: 100)
na.action the action to perform on NA
... Other arguments that can be passed to qtSNE

Details

When the initial_config argument is specified, the algorithm will automatically enter the final momentum stage. This stage has less large scale adjustment to the embedding, and is intended for small scale tweaking of positioning. This can greatly speed up the generation of embeddings for various similar X datasets, while also preserving overall embedding orientation.

Value

qtSNE gives out an S4 object which is a LIST with components

dimRed Matrix containing the new representations for the objects after qtSNE
ckernel The kernel function used

Author(s)

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qtSNE-class

References


Examples

```r
## Not run:
# use iris data set
data(iris)
testset <- sample(1:150,20)
train <- as.matrix(iris[,1:4])

colors = rainbow(length(unique(iris$Species)))
names(colors) = unique(iris$Species)

# for matrix
ecb = function(x,y){
  plot(x,t='n');
  text(x,labels=iris$Species, col=colors[iris$Species])
}

kpc2 <- qtSNE(train, kernel = "rbfbase", qpar = list(sigma=1,q=0.8),
              epoch_callback = ecb, perplexity=10, max_iter = 500)

## End(Not run)
```

qtSNE-class  

Class "qtSNE"

Description

An S4 Class for qtSNE.

Details

The qtSNE is a method that uses Qkernel t-Distributed Stochastic Neighborhood Embedding between the distance matrices in high and low-dimensional space to embed the data. The method is very well suited to visualize complex structures in low dimensions.

Objects from the Class

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

Slots

- `dimRed` Matrix containing the new representations for the objects after qtSNE
- `cndkernf` The kernel function used
Method

- `dimRed signature(object="qtSNE")`: return a new representation matrix
- `cndkernf signature(object="qtSNE")`: return the kernel used

Author(s)

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References


See Also

- `qtSNE`

Examples

```r
## Not run:

# use iris data set
data(iris)
testset <- sample(1:150,20)
train <- as.matrix(iris[,1:4])

colors = rainbow(length(unique(iris$Species)))
names(colors) = unique(iris$Species)

# for matrix
ecb = function(x,y){
  plot(x,t='n');
  text(x,labels=iris$Species, col=colors[iris$Species])
}
kpc2 <- qtSNE(train, kernel = "rbfbase", qpar = list(sigma=1,q=0.8),
  epoch_callback = ecb, perplexity=10, max_iter = 500)

#cndernf
cndkernf(kpc2)

#dimRed
plot(dimRed(kpc2),col=train)

## End(Not run)
```
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