Package ‘FNN’

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R topics documented:
crossentropy ...................................................... 2
entropy .......................................................... 3
get.knn ............................................................ 4
KL.dist ............................................................ 5
KL.divergence ..................................................... 6
knn ................................................................. 8
knn.cv ............................................................. 9
knn.dist .......................................................... 10
knn.index ........................................................ 11
knn.reg ........................................................... 13
mutinfo ........................................................... 14
ownn ............................................................... 15
print.knnReg ..................................................... 16
**crossentropy**

**Description**

KNN Cross Entropy Estimators.

**Usage**

```r
crossentropy(X, Y, k=10, algorithm=c("kd_tree", "cover_tree", "brute"))
```

**Arguments**

- `X`: an input data matrix.
- `Y`: an input data matrix.
- `k`: the maximum number of nearest neighbors to search. The default value is set to 10.
- `algorithm`: nearest neighbor search algorithm.

**Details**

If \( p(x) \) and \( q(x) \) are two continuous probability density functions, then the cross-entropy of \( p \) and \( q \) is defined as \( H(p; q) = E_p[-\log q(x)] \).

**Value**

a vector of length \( k \) for crossentropy estimates using \( 1:k \) nearest neighbors, respectively.

**Author(s)**

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

**References**

entropy

Shannon Entropy

Description

KNN Shannon Entropy Estimators.

Usage

```r
entropy(X, k = 10, algorithm = c("kd_tree", "brute"))
```

Arguments

- `X` an input data matrix.
- `k` the maximum number of nearest neighbors to search. The default value is set to 10.
- `algorithm` nearest neighbor search algorithm.

Value

a vector of length `k` for entropy estimates using `1:k` nearest neighbors, respectively.

Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

References


get.knn

**Search Nearest Neighbors**

### Description

Fast k-nearest neighbor searching algorithms including a kd-tree, cover-tree and the algorithm implemented in class package.

### Usage

```r
get.knn(data, k=10, algorithm=c("kd_tree", "cover_tree", "CR", "brute"))
get.knnx(data, query, k=10, algorithm=c("kd_tree", "cover_tree", "CR", "brute"))
```

### Arguments

- **data**: an input data matrix.
- **query**: a query data matrix.
- **algorithm**: nearest neighbor searching algorithm.
- **k**: the maximum number of nearest neighbors to search. The default value is set to 10.

### Details

The **cover tree** is O(n) space data structure which allows us to answer queries in the same O(log(n)) time as **kd tree** given a fixed intrinsic dimensionality. Templated code from [https://hunch.net/~jl/projects/cover_tree/cover_tree.html](https://hunch.net/~jl/projects/cover_tree/cover_tree.html) is used.

The **kd tree** algorithm is implemented in the Approximate Near Neighbor (ANN) C++ library (see [http://www.cs.umd.edu/~mount/ANN/](http://www.cs.umd.edu/~mount/ANN/)). The exact nearest neighbors are searched in this package.

The **CR** algorithm is the VR using distance \(1-x'y\) assuming \(x\) and \(y\) are unit vectors. The **brute** algorithm searches linearly. It is a naive method.

### Value

A list contains:

- **nn.index**: an n x k matrix for the nearest neighbor indice.
- **nn.dist**: an n x k matrix for the nearest neighbor Euclidean distances.

### Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>
References


See Also

`nn2` in `RANN`, `ann` in `yaImpute` and `knn` in `class`.

Examples

```r
data<- query<- cbind(1:10, 1:10)

get.knn(data, k=5)
get.knn(data, query, k=5)
get.knn(data, query, k=5, algo="kd_tree")

th<- runif(10, min=0, max=2*pi)
data2<- cbind(cos(th), sin(th))
get.knn(data2, k=5, algo="CR")
```

---

**KL.dist**  
*Kullback-Leibler Divergence*

**Description**

Compute Kullback-Leibler symmetric distance.

**Usage**

```r
KL.dist(X, Y, k = 10, algorithm=c("kd_tree", "cover_tree", "brute"))
KLx.dist(X, Y, k = 10, algorithm="kd_tree")
```

**Arguments**

- `X`  
  An input data matrix.

- `Y`  
  An input data matrix.

- `k`  
  The maximum number of nearest neighbors to search. The default value is set to 10.

- `algorithm`  
  nearest neighbor search algorithm.
Details
Kullback-Leibler distance is the sum of divergence $q(x)$ from $p(x)$ and $p(x)$ from $q(x)$.

KL.* versions return distances from C code to R but KLx.* do not.

Value
Return the Kullback-Leibler distance between $X$ and $Y$.

Author(s)
Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

References

See Also
KL.divergence.

Examples
```r
set.seed(1000)
X<- rexp(10000, rate=0.2)
Y<- rexp(10000, rate=0.4)

KL.dist(X, Y, k=5)
KLx.dist(X, Y, k=5)
#theoretical distance = (0.2-0.4)^2/(0.2*0.4) = 0.5
```
**KL.divergence**

**Arguments**
- **X**  
  An input data matrix.
- **Y**  
  An input data matrix.
- **k**  
  The maximum number of nearest neighbors to search. The default value is set to 10.
- **algorithm**  
  nearest neighbor search algorithm.

**Details**

If \( p(x) \) and \( q(x) \) are two continuous probability density functions, then the Kullback-Leibler divergence of \( q \) from \( p \) is defined as \( E_p[\log \frac{p(x)}{q(x)}] \).

\( \text{KL}.\ast \) versions return divergences from C code to R but \( \text{KLx}.\ast \) do not.

**Value**

Return the Kullback-Leibler divergence from \( X \) to \( Y \).

**Author(s)**

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

**References**


**See Also**

- **KL.dist**

**Examples**

```r
set.seed(1000)
X <- rexp(10000, rate=0.2)
Y <- rexp(10000, rate=0.4)
KL.divergence(X, Y, k=5)
#theoretical divergence = log(0.2/0.4)+(0.4-0.2)-1 = 1-log(2) = 0.307
```
**knn**

**k-Nearest Neighbour Classification**

**Description**

k-nearest neighbour classification for test set from training set. For each row of the test set, the k nearest (in Euclidean distance) training set vectors are found, and the classification is decided by majority vote, with ties broken at random. If there are ties for the kth nearest vector, all candidates are included in the vote.

**Usage**

```r
knn(train, test, cl, k = 1, prob = FALSE, algorithm=c("kd_tree", "cover_tree", "brute"))
```

**Arguments**

- `train` matrix or data frame of training set cases.
- `test` matrix or data frame of test set cases. A vector will be interpreted as a row vector for a single case.
- `cl` factor of true classifications of training set.
- `k` number of neighbours considered.
- `prob` if this is true, the proportion of the votes for the winning class are returned as attribute `prob`.
- `algorithm` nearest neighbor search algorithm.

**Value**

factor of classifications of test set. `doubt` will be returned as `NA`.

**Author(s)**

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

**References**


**See Also**

`ownn`, `knn.cv` and `knn` in `class`. 
Examples

data(iris3)
train <- rbind(iris3[1:25,,1], iris3[1:25,,2], iris3[1:25,,3])
test <- rbind(iris3[26:50,,1], iris3[26:50,,2], iris3[26:50,,3])
c1 <- factor(c(rep("s",25), rep("c",25), rep("v",25)))
knn(train, test, cl, k = 3, prob=TRUE)
attributes(.Last.value)

knn.cv

k-Nearest Neighbour Classification Cross-Validation

Description

k-nearest neighbour classification cross-validation from training set.

Usage

knn.cv(train, cl, k = 1, prob = FALSE, algorithm=c("kd_tree",  
"cover_tree", "brute"))

Arguments

train matrix or data frame of training set cases.
cl factor of true classifications of training set
k number of neighbours considered.
prob if this is true, the proportion of the votes for the winning class are returned as  
attribute prob.
algorithm nearest neighbor search algorithm.

Details

This uses leave-one-out cross validation. For each row of the training set train, the k nearest  
(in Euclidean distance) other training set vectors are found, and the classification is decided by  
majority vote, with ties broken at random. If there are ties for the kth nearest vector, all candidates  
are included in the vote.

Value

factor of classifications of training set. doubt will be returned as NA. distances and indice of k  
nearest neighbors are also returned as attributes.

Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>
References


See Also

knn and knn.cv in class.

Examples

data(iris3)
train <- rbind(iris3[,1], iris3[,2], iris3[,3])
c1 <- factor(c(rep("s",50), rep("c",50), rep("v",50)))
knncv(train, c1, k = 3, prob = TRUE)
attributes(.Last.value)

---

knn.dist

**k Nearest Neighbor Distances**

Description

Fast k-nearest neighbor distance searching algorithms.

Usage

knn.dist(data, k=10, algorithm=c("kd_tree", "cover_tree", "CR", "brute"))

knnx.dist(data, query, k=10, algorithm=c("kd_tree", "cover_tree", "CR", "brute"))

Arguments

data an input data matrix.
query a query data matrix.
algorithm nearest neighbor searching algorithm.
k the maximum number of nearest neighbors to search. The default value is set to 10.

Value

return the Euclidean distances of k nearest neighbors.

Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>
**knn.index**

**Search Nearest Neighbors**

**Description**

Fast k-nearest neighbor searching algorithms including a kd-tree, cover-tree and the algorithm implemented in class package.

**Usage**

```r
knn.index(data, k=10, algorithm=c("kd_tree", "cover_tree", "CR", "brute"))
knnx.index(data, query, k=10, algorithm=c("kd_tree", "cover_tree", "CR", "brute"))
```

**References**


**See Also**

`get.knn` and `knn.index`.

**Examples**

```r
if(require(mvtnorm))
{
  sigma<- function(v, r, p)
  {
    V<- matrix(r^2, ncol=p, nrow=p)
    diag(V)<- 1
    V*v
  }
  X<- rmvnorm(1000, mean=rep(0, 20), sigma(1, .5, 20))
  print(system.time(knn.dist(X)) )
  print(system.time(knn.dist(X, algorithm = "kd_tree")))
}
```
**Arguments**

- **data**: an input data matrix.
- **query**: a query data matrix.
- **algorithm**: nearest neighbor searching algorithm.
- **k**: the maximum number of nearest neighbors to search. The default value is set to 10.

**Value**

return the indice of k nearest neighbors.

**Author(s)**

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

**References**


**See Also**

- `knn.dist` and `get.knn`.

**Examples**

```r
data<- query<- cbind(1:10, 1:10)
knn.index(data, k=5)
knnx.index(data, query, k=5)
knnx.index(data, query, k=5, algo="kd_tree")
```
### knn.reg

**k Nearest Neighbor Regression**

#### Description

k-nearest neighbor regression

#### Usage

```r
knn.reg(train, test = NULL, y, k = 3, algorithm=c("kd_tree", "cover_tree", "brute"))
```

#### Arguments

- `train`: matrix or data frame of training set cases.
- `test`: matrix or data frame of test set cases. A vector will be interpreted as a row vector for a single case. If not supplied, cross-validation will be done.
- `y`: response of each observation in the training set.
- `k`: number of neighbours considered.
- `algorithm`: nearest neighbor search algorithm.

#### Details

If `test` is not supplied, Leave one out cross-validation is performed and *R-square* is the predicted R-square.

#### Value

`knn.reg` returns an object of class "knnReg" or "knnRegCV" if `test` data is not supplied.

The returned object is a list containing at least the following components:

- `call`: the match call.
- `k`: number of neighbours considered.
- `n`: number of predicted values, either equals test size or train size.
- `pred`: a vector of predicted values.
- `residuals`: predicted residuals. NULL if `test` is supplied.
- `PRESS`: the sums of squares of the predicted residuals. NULL if `test` is supplied.
- `R2Pred`: predicted R-square. NULL if `test` is supplied.

#### Note

The code for “VR” nearest neighbor searching is taken from `class` source
Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

See Also

knn.

Examples

```r
if(require(chemometrics)){
data(PAC);
pac.knn<- knn.reg(PAC$X, y=PAC$y, k=3);

   plot(PAC$y, pac.knn$pred, xlab="y", ylab=expression(hat(y)))
}
```

Description

KNN Mutual Information Estimators.

Usage

```r
mutinfo(X, Y, k=10, direct=TRUE)
```

Arguments

- `X`: an input data matrix.
- `Y`: an input data matrix.
- `k`: the maximum number of nearest neighbors to search. The default value is set to 10.
- `direct`: Directly compute or via entropies.

Details

The direct computation is based on the first estimator of A. Kraskov, H. Stogbauer and P.Grassberger (2004) and the indirect computation is done via entropy estimates, i.e., \( I(X, Y) = H(X) + H(Y) - H(X, Y) \). The direct method has smaller bias and variance but the indirect method is faster, see Evans (2008).

Value

For direct method, one mutual information estimate; For indirect method, a vector of length `k` for mutual information estimates using 1: `k` nearest neighbors, respectively.
Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>

References


Optimal Weighted Nearest Neighbor Classification

Description

This function implements Samworth’s optimal weighting scheme for k nearest neighbor classification. The performance improvement is greatest when the dimension is 4 as reported in the reference.

Usage

ownn(train, test, cl, testcl=NULL, k = NULL, prob = FALSE, 
algorithm=c("kd_tree", "cover_tree", "brute"))

Arguments

train matrix or data frame of training set cases.

test matrix or data frame of test set cases. A vector will be interpreted as a row vector for a single case.

cl factor of true classifications of training set.

testcl factor of true classifications of testing set for error rate calculation.

k number of neighbours considered, chosen by 5-fold cross-validation if not supplied.

prob if this is true, the proportion of the weights for the winning class are returned as attribute prob.

algorithm nearest neighbor search algorithm.

Value

a list includes k, predictions by ordinary knn, optimal weighted knn and bagged knn, and accuracies if class labels of test data set are given.

Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>
References


See Also

`knn` and `knn` in `class`.

Examples

data(iris3)
train <- rbind(iris3[1:25,,1], iris3[1:25,,2], iris3[1:25,,3])
test <- rbind(iris3[26:50,,1], iris3[26:50,,2], iris3[26:50,,3])
cl <- factor(c(rep("s",25), rep("c",25), rep("v",25)))
testcl <- factor(c(rep("s",25), rep("c",25), rep("v",25)))
out <- ownn(train, test, cl, testcl)
out

print.knnReg  Print Method for KNN Regression

Description

Print method for KNN regression.

Usage

## S3 method for class 'knnReg'
print(x, ...)
## S3 method for class 'knnRegCV'
print(x, ...)

Arguments

x  
a knnReg or knnRegCV object.
...
   Additonal print arguments.

Author(s)

Shengqiao Li. To report any bugs or suggestions please email: <lishengqiao@yahoo.com>
Index

* classif
  knn, 8
  knn.cv, 9
  ownn, 15
* manip
  crossentropy, 2
  entropy, 3
  get.knn, 4
  KL.dist, 5
  KL.divergence, 6
  knn.dist, 10
  knn.index, 11
  mutinfo, 14
* nonparametric
  knn, 8
  knn.cv, 9
  knn.reg, 13
  ownn, 15
* print
  print.knnReg, 16
* regression
  knn.reg, 13

crossentropy, 2

entropy, 3

get.knn, 4, 11, 12
get.knmx (get.knn), 4

KL.dist, 5, 7
KL.divergence, 6, 6
KLx.dist (KL.dist), 5
KLx.divergence (KL.divergence), 6
knn, 5, 8, 8, 10, 14, 16
knn.cv, 8, 9, 10
knn.dist, 10, 12
knn.index, 11, 11
knn.reg, 13
knnx.dist (knn.dist), 10

knnx.index (knn.index), 11

mutinfo, 14

ownn, 8, 15

print.knnReg, 16
print.knnRegCV (print.knnReg), 16

17