Package ‘sda’
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Description Provides an efficient framework for
     high-dimensional linear and diagonal discriminant analysis with
     variable selection. The classifier is trained using James-Stein-type
     shrinkage estimators and predictor variables are ranked using
     correlation-adjusted t-scores (CAT scores). Variable selection error
     is controlled using false non-discovery rates or higher criticism.
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The sda Package

Description

This package performs linear discriminant analysis (LDA) and diagonal discriminant analysis (DDA) with variable selection using correlation-adjusted t (CAT) scores.

The classifier is trained using James-Stein-type shrinkage estimators. Variable selection is based on ranking predictors by CAT scores (LDA) or t-scores (DDA). A cutoff is chosen by false non-discovery rate (FNDR) or higher criticism (HC) thresholding.

This approach is particularly suited for high-dimensional classification with correlation among predictors. For details see Zuber and Strimmer (2009) and Ahdesmäki and Strimmer (2010).

Typically the functions in this package are applied in three steps:

- Step 1: feature selection with \texttt{sda.ranking},
- Step 2: training the classifier with \texttt{sda}, and
- Step 3: classification using \texttt{predict.sda}.

The accompanying web site (see below) provides example R scripts to illustrate the functionality of this package.

Author(s)

Miika Ahdesmäki, Verena Zuber and Korbinian Strimmer (\url{http://strimmerlab.org/})

References


See website: \url{http://strimmerlab.org/software/sda/}

See Also

\texttt{catscore}, \texttt{sda.ranking}, \texttt{sda.predict.sda}. 
catscore

Estimate CAT Scores and t-Scores

Description

catscore computes CAT scores (correlation-adjusted t-scores) between the group centroids and the pooled mean.

Usage

catscore(Xtrain, L, lambda, lambda.var, lambda.freqs, diagonal=FALSE, verbose=TRUE)

Arguments

- **Xtrain**: A matrix containing the training data set. Note that the rows correspond to observations and the columns to variables.
- **L**: A factor with the class labels of the training samples.
- **lambda**: Shrinkage intensity for the correlation matrix. If not specified it is estimated from the data. lambda=0 implies no shrinkage and lambda=1 complete shrinkage.
- **lambda.var**: Shrinkage intensity for the variances. If not specified it is estimated from the data. lambda.var=0 implies no shrinkage and lambda.var=1 complete shrinkage.
- **lambda.freqs**: Shrinkage intensity for the frequencies. If not specified it is estimated from the data. lambda.freqs=0 implies no shrinkage (i.e. empirical frequencies) and lambda.freqs=1 complete shrinkage (i.e. uniform frequencies).
- **diagonal**: for diagonal=FALSE (the default) CAT scores are computed; otherwise with diagonal=TRUE t-scores.
- **verbose**: Print out some info while computing.

Details

CAT scores generalize conventional t-scores to account for correlation among predictors (Zuber and Strimmer 2009). If there is no correlation then CAR scores reduce to t-scores. The squared CAR scores provide a decomposition of Hotelling’s $T^2$ statistic.

CAT scores for two classes are described in Zuber and Strimmer (2009), for the multi-class case see Ahdesmäki and Strimmer (2010).

The scale factors for t-scores and CAT-scores are computed from the estimated frequencies (for empirical scale factors set lambda.freqs=0).

Value

catscore returns a matrix containing the cat score (or t-score) between each group centroid and the pooled mean for each feature.
Author(s)


References


See Also

sda.ranking, carscore.

Examples

# load sda library
library("sda")

# training data #
# prostate cancer set
data(singh2002)

# training data
Xtrain = singh2002$x
Ytrain = singh2002$y
dim(Xtrain)

tstat = carscore(Xtrain, Ytrain, diagonal=TRUE)
dim(tstat)
tstat[1:10,]

cat = carscore(Xtrain, Ytrain, diagonal=FALSE)
dim(cat)
cat[1:10,]
centroids

Group Centroids and (Pooled) Variances

Description

centroids computes group centroids, the pooled mean and pooled variance, and optionally the group specific variances.

Usage

centroids(x, L, lambda.var, lambda.freqs, var.groups=FALSE, centered.data=FALSE, verbose=TRUE)

Arguments

- **x**: A matrix containing the data set. Note that the rows are sample observations and the columns are variables.
- **L**: A factor with the group labels.
- **lambda.var**: Shrinkage intensity for the variances. If not specified it is estimated from the data, see details below. lambda.var=0 implies no shrinkage and lambda.var=1 complete shrinkage.
- **lambda.freqs**: Shrinkage intensity for the frequencies. If not specified it is estimated from the data. lambda.freqs=0 implies no shrinkage (i.e. empirical frequencies) and lambda.freqs=1 complete shrinkage (i.e. uniform frequencies).
- **var.groups**: Estimate group-specific variances.
- **centered.data**: Return column-centered data matrix.
- **verbose**: Provide some messages while computing.

Details

As estimator of the variance we employ `var.shrink` as described in Opgen-Rhein and Strimmer (2007). For the estimates of frequencies we rely on `freqs.shrink` as described in Hausser and Strimmer (2009). Note that the pooled mean is computed using the estimated frequencies.

Value

centroids returns a list with the following components:

- **samples**: a vector containing the samples sizes in each group,
- **freqs**: a vector containing the estimated frequency in each group,
- **means**: the group means and the pooled mean,
- **variances**: the group-specific and the pooled variances, and
- **centered.data**: a matrix containing the centered data.
Author(s)

Korbinian Strimmer (http://strimmerlab.org).

See Also

var.shrink, powcor.shrink.

Examples

```r
# load sda library
library("sda")

## prepare data set
data(iris)  # good old iris data
X = as.matrix(iris[,1:4])
Y = iris[,5]

## estimate centroids and empirical pooled variances
centroids(X, Y, lambda.var=0)

## also compute group-specific variances
centroids(X, Y, var.groups=TRUE, lambda.var=0)

## use shrinkage estimator for the variances
centroids(X, Y, var.groups=TRUE)

## return centered data
xc = centroids(X, Y, centered.data=TRUE)$centered.data
apply(xc, 2, mean)

## useful, e.g., to compute the inverse pooled correlation matrix
powcor.shrink(xc, alpha=-1)
```

---

khan2001  
Childhood Cancer Study of Khan et al. (2001)

Description

Gene expression data (2308 genes for 88 samples) from the microarray study of Khan et al. (2001).

Usage

data(khan2001)
Format

khan2001$x is a 88 x 2308 matrix containing the expression levels. Note that rows correspond to samples, and columns to genes. The row names are the original image IDs, and the column names the original probe labels.

khan2001$y is a factor containing the diagnosis for each sample ("BL", "EWS", "NB", "non-SRBCT", "RMS").

khan2001$descr provides some annotation for each gene.

Details

This data set contains measurements of the gene expression of 2308 genes for 88 observations: 29 cases of Ewing sarcoma (EWS), 11 cases of Burkitt lymphoma (BL), 18 cases of neuroblastoma (NB), 25 cases of rhabdomyosarcoma (RMS), and 5 other (non-SRBCT) samples.

Source

The data are described in Khan et al. (2001). Note that the values in khan.data$x are logarithmized (using natural log) for normalization.

References


Examples

# load sda library
library("sda")

# load full Khan et al (2001) data set
data(khan2001)
dim(khan2001$x) # 88 2308
hist(khan2001$x)
khan2001$y # 5 levels

# data set containing the SRBCT samples
get.srbct = function()
{
  data(khan2001)
  idx = which( khan2001$y == "non-SRBCT" )
  x = khan2001$x[-idx,]
  y = factor(khan2001$y[-idx])
  descr = khan2001$descr[-idx]

  list(x=x, y=y, descr=descr)
}

srbct = get.srbct()
dim(srbct$x) # 83 2308
hist(srbct$x)
predict.sda

Srbct$y # 4 levels

predict.sda  Shrinkage Discriminant Analysis 3: Prediction Step

Description

predict.sda performs class prediction.

Usage

## S3 method for class 'sda'
predict(object, Xtest, verbose=TRUE, ...)

Arguments

- object: An sda fit object obtained from the function sda.
- Xtest: A matrix containing the test data set. Note that the rows correspond to observations and the columns to variables.
- verbose: Report shrinkage intensities (sda) and number of used features (predict.sda).
- ...: Additional arguments for generic predict.

Value

predict.sda predicts class probabilities for each test sample and returns a list with two components:

- class: a factor with the most probable class assignment for each test sample, and
- posterior: a matrix containing the respective class posterior probabilities.

Author(s)

Miiika Ahdesmäki and Korbinian Strimmer ([http://strimmerlab.org](http://strimmerlab.org)).

See Also

sda, sda.ranking.

Examples

# see the examples at the "sda" help page
Shrinkage Discriminant Analysis 2: Training Step

Description

`sda` trains a LDA or DDA classifier using James-Stein-type shrinkage estimation.

Usage

`sda(Xtrain, L, lambda, lambda.var, lambda.freqs, diagonal=FALSE, verbose=TRUE)`

Arguments

- **Xtrain**: A matrix containing the training data set. Note that the rows correspond to observations and the columns to variables.
- **L**: A factor with the class labels of the training samples.
- **lambda**: Shrinkage intensity for the correlation matrix. If not specified it is estimated from the data. `lambda=0` implies no shrinkage and `lambda=1` complete shrinkage.
- **lambda.var**: Shrinkage intensity for the variances. If not specified it is estimated from the data. `lambda.var=0` implies no shrinkage and `lambda.var=1` complete shrinkage.
- **lambda.freqs**: Shrinkage intensity for the frequencies. If not specified it is estimated from the data. `lambda.freqs=0` implies no shrinkage (i.e. empirical frequencies) and `lambda.freqs=1` complete shrinkage (i.e. uniform frequencies).
- **diagonal**: Chooses between LDA (default, diagonal=FALSE) and DDA (diagonal=TRUE).
- **verbose**: Print out some info while computing.

Details

In order to train the LDA or DDA classifier, three separate shrinkage estimators are employed:

- **class frequencies**: the estimator `freqs.shrink` from Hausser and Strimmer (2008),
- **variances**: the estimator `var.shrink` from Opgen-Rhein and Strimmer (2007),
- **correlations**: the estimator `cor.shrink` from Schäfer and Strimmer (2005).

Note that the three corresponding regularization parameters are obtained analytically without resorting to computer intensive resampling.
Value

sda trains the classifier and returns an sda object with the following components needed for the subsequent prediction:

- **regularization**: a vector containing the three estimated shrinkage intensities,
- **freqs**: the estimated class frequencies,
- **alpha**: vector containing the intercepts used for prediction,
- **beta**: matrix containing the coefficients used for prediction.

Author(s)


References


See Also

predict.sda, sda.ranking, freqs.shrink, var.shrink, invcor.shrink.

Examples

```r
# load sda library
library("sda")

# data set containing the SRBCT samples
get.srbct = function()
{
  data(khan2001)
  idx = which( khan2001$y == "non-SRBCT" )
  x = khan2001$x[-idx,]
  y = factor(khan2001$y[-idx])
  descr = khan2001$descr[-idx]

  list(x=x, y=y, descr=descr)
}
srbct = get.srbct()

# training data
Xtrain = srbct$x[1:63,]
Ytrain = srbct$y[1:63]
Xtest = srbct$x[64:83,]
Ytest = srbct$y[64:83]
```
sda.ranking

### Shrinkage Discriminant Analysis I: Predictor Ranking

**Description**

sda.ranking determines a ranking of predictors by computing CAT scores (correlation-adjusted t-scores) between the group centroids and the pooled mean.

plot.sda.ranking provides a graphical visualization of the top ranking features.

**Usage**

```r
sda.ranking(Xtrain, L, lambda, lambda.var, lambda.freqs, 
  ranking.score=c("entropy", "avg", "max"), 
  diagonal=FALSE, fdr=TRUE, plot.fdr=FALSE, verbose=TRUE)
```

**Arguments**

- `Xtrain`: A matrix containing the training data set. Note that the rows correspond to observations and the columns to variables.
- `L`: A factor with the class labels of the training samples.
- `lambda`: Shrinkage intensity for the correlation matrix. If not specified it is estimated from the data. `lambda=0` implies no shrinkage and `lambda=1` complete shrinkage.
**sda.ranking**

- **lambda.var**: Shrinkage intensity for the variances. If not specified it is estimated from the data. \( \lambda_{\text{var}} = 0 \) implies no shrinkage and \( \lambda_{\text{var}} = 1 \) complete shrinkage.

- **lambda.freqs**: Shrinkage intensity for the frequencies. If not specified it is estimated from the data. \( \lambda_{\text{freqs}} = 0 \) implies no shrinkage (i.e. empirical frequencies) and \( \lambda_{\text{freqs}} = 1 \) complete shrinkage (i.e. uniform frequencies).

- **diagonal**: Chooses between LDA (default, \( \text{diagonal} = \text{FALSE} \)) and DDA (\( \text{diagonal} = \text{TRUE} \)).

- **ranking.score**: how to compute the summary score for each variable from the CAT scores of all classes - see Details.

- **fdr**: compute FDR values and HC scores for each feature.

- **plot.fdr**: Show plot with estimated FDR values.

- **verbose**: Print out some info while computing.

- **x**: An "sda.ranking" object – this is produced by the `sda.ranking()` function.

- **top**: The number of top-ranking features shown in the plot (default: 40).

- **arrow.col**: Color of the arrows in the plot (default is "blue").

- **zeroaxis.col**: Color for the center zero axis (default is "red").

- **ylab**: Label written next to feature list (default is "features").

- **main**: Main title (if missing, "The", top, "Top Ranking Features" is used).

- **...**: Other options passed on to generic `plot()`.

**Details**

For each predictor variable and centroid a shrinkage CAT scores of the mean versus the pooled mean is computed. If there are only two classes the CAT score vs. the pooled mean reduces to the CAT score between the two group means. Moreover, in the diagonal case (LDA) the (shrinkage) CAT score reduces to the (shrinkage) t-score.

The overall ranking of a feature is determine by computing a summary score from the CAT scores. This is controlled by the option `ranking.score`. The default setting (`ranking.score = "entropy"`) uses mutual information between the response and the respective predictors (`ranking.score`) for ranking. This is equivalent to a weighted sum of squared CAT scores across the classes. Another possibility is to employ the average of the squared CAT scores for ranking (as suggested in Ahdesmäki and Strimmer 2010) by setting `ranking.score = "avg"`. A third option is to use the maximum of the squared CAT scores across groups (similarly as in the PAM algorithm) via setting `ranking.score = "max"`. Note that in the case of two classes all three options are equivalent and lead to identical scores. Thus, the choice of `ranking.score` is important only in the multi-class setting. In the two-class case the features are simply ranked according to the (shrinkage) squared CAT-scores (or t-scores, if there is no correlation among predictors).

The current default approach is to use ranking by mutual information (i.e. relative entropy between full model vs. model without predictor) and to use shrinkage estimators of frequencies. In order to reproduce exactly the ranking computed by previous versions (1.1.0 to 1.3.0) of the sda package set the options `ranking.score = "avg"` and \( \lambda_{\text{freqs}} = 0 \).

Calling `sda.ranking` is step 1 in a classification analysis with the sda package. Steps 2 and 3 are `sda` and `predict.sda`.

sda.ranking

Value

sda.ranking returns a matrix with the following columns:

- **idx**: original feature number
- **score**: sum of the squared CAT scores across groups - this determines the overall ranking of a feature
- **cat**: for each group and feature the cat score of the centroid versus the pooled mean

If fdr=TRUE then additionally local false discovery rate (FDR) values as well as higher criticism (HC) scores are computed for each feature (using fdrtool).

Author(s)


References


See Also

catscore, sda, predict.sda.

Examples

```r
# load sda library
library("sda")

# training data #

# prostate cancer set
data(singh2002)

# training data
Xtrain = singh2002$x
Ytrain = singh2002$y

# feature ranking (diagonal covariance) #
```
# ranking using t-scores (DDA)
ranking.DDA = sda.ranking(Xtrain, Ytrain, diagonal=TRUE)
ranking.DDA[1:10,]

# plot t-scores for the top 40 genes
plot(ranking.DDA, top=40)

# number of features with local FDR < 0.8
# (i.e. features useful for prediction)
sum(ranking.DDA[,"lfdr"] < 0.8)

# number of features with local FDR < 0.2
# (i.e. significant non-null features)
sum(ranking.DDA[,"lfdr"] < 0.2)

# optimal feature set according to HC score
plot(ranking.DDA[,"HC"], type="l")
which.max( ranking.DDA[1:1000,"HC"] )

# ranking using CAT-scores (LDA)
ranking.LDA = sda.ranking(Xtrain, Ytrain, diagonal=FALSE)
ranking.LDA[1:10,]

# plot t-scores for the top 40 genes
plot(ranking.LDA, top=40)

# number of features with local FDR < 0.8
# (i.e. features useful for prediction)
sum(ranking.LDA[,"lfdr"] < 0.8)

# number of features with local FDR < 0.2
# (i.e. significant non-null features)
sum(ranking.LDA[,"lfdr"] < 0.2)

# optimal feature set according to HC score
plot(ranking.LDA[,"HC"], type="l")
which.max( ranking.LDA[1:1000,"HC"] )

# feature ranking (full covariance) #

Description
Gene expression data (6033 genes for 102 samples) from the microarray study of Singh et al. (2002).
Usage

data(singh2002)

Format

singh2002$x is a 102 x 6033 matrix containing the expression levels. The rows contain the samples and the columns the genes.
singh2002$y is a factor containing the diagnosis for each sample ("cancer" or "healthy").

Details

This data set contains measurements of the gene expression of 6033 genes for 102 observations: 52 prostate cancer patients and 50 healthy men.

Source

The data are described in Singh et al. (2001) and are provided in exactly the form as used by Efron (2008).

References


Examples

# load sda library
library("sda")

# load Singh et al (2001) data set
data(singh2002)
dim(singh2002$x) # 102 6033
hist(singh2002$x)
singh2002$y # 2 levels
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