Package 'BOSSreg'

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Title Best Orthogonalized Subset Selection (BOSS)
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Description Best orthogonalized subset selection (BOSS) is a least-squares (LS) based subset selec-
      tion method, that performs best subset selection upon an orthogonalized basis of ordered predic-
      tors, with the computational effort of a single ordinary LS fit. This package provides a highly op-
      timized implementation of BOSS and estimates a heuristic degrees of free-
      dom for BOSS, which can be plugged into an information criterion (IC) such as AICc in or-
      der to select the subset from candidates. It provides various choices of IC, includ-
      ing AIC, BIC, AICc, Cp and GCV. It also implements the forward stepwise selec-
      tion (FS) with no additional computational cost, where the subset of FS is selected via cross-
      validation (CV). CV is also an option for BOSS. For details see: Tian, Hurvich and Si-
      monoff (2019), On the Use of Information Criteria for Subset Selection in Least Squares Regres-
      sion, <arXiv:1911.10191>.
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URL https://github.com/sentian/BOSSreg

BugReports https://github.com/sentian/BOSSreg/issues

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Best Orthogonalized Subset Selection (BOSS).

Description

- Compute the solution path of BOSS and forward stepwise selection (FS).
- Compute various information criteria based on a heuristic degrees of freedom (hdf) that can serve as the selection rule to choose the subset given by BOSS. Only work when n>p.

Usage

```
boss(x, y, intercept = TRUE, hdf.ic.boss = TRUE, mu = NULL,
    sigma = NULL, ...)
```

Arguments

X	A matrix of predictors, with $nrow(x) = length(y) = n$ observations and $ncol(x) = p$ predictors. Intercept shall NOT be included.
у	A vector of response variable, with length(y)=n.
intercept	Logical, whether to include an intercept term. Default is TRUE.
hdf.ic.boss	Logical, whether to calculate the heuristic degrees of freedom (hdf) and information criteria (IC) for BOSS. IC includes AIC, BIC, AICc, BICc, GCV, Cp. Note that if n<=p, hdf.ic.boss=FALSE no matter what. Default is TRUE.
mu	True mean vector, used in the calculation of hdf. Default is NULL, and is estimated via least-squares (LS) regression of y upon x .
sigma	True standard deviation of the error, used in the calculation of hdf. Default is NULL, and is estimated via least-squares (LS) regression of y upon x.
	Extra parameters to allow flexibility. Currently none allows or requires, just for the convinience of call from other parent functions like cv.boss.

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Details

This function computes the full solution path given by BOSS and FS on a given dataset (x,y) with n observations and p predictors. In the case where n>p, it also calculates the heuristic degrees of freedom for BOSS, and various information criteria, which can further be used to select the subset from the candidates. Please refer to the Vignette for implementation details and Tian et al. (2019) for methodology details (links are given below).

Value

- beta_fs: A matrix of regression coefficients for all the subsets given by FS, from a null model until stop, with nrow=p and ncol=min(n,p)+1, where min(n,p) is the maximum number of steps performed.
- beta_boss: A matrix of regression coefficients for all the subsets given by BOSS, with nrow=p and ncol=min(n,p)+1. Note that unlike beta_fs and due to the nature of BOSS, the number of non-zero components in columns of beta_boss may not be unique, i.e. there maybe multiple columns corresponding to the same size of subset.
- steps_x: A vector of numbers representing which predictor joins at each step, with length(steps)=min(n,p).
 The ordering is determined by the partial correlation between a predictor x_j and the response y.
- steps_q: A vector of numbers representing which predictor joins at each step in the orthogonal basis, with length(steps)=min(n,p). BOSS takes the ordered predictors (ordering given in steps_x) and performs best subset regression upon their orthogonal basis, which is essentially ordering the orthogonalized predictors by their marginal correlations with the response y. For example, steps_q=c(2,1) indicates that the orthogonal basis of x_2 joins first.
- hdf_boss: A vector of heuristic degrees of freedom (hdf) for BOSS, with length(hdf_boss)=p+1. Note that hdf_boss=NULL if n<=p or hdf.ic.boss=FALSE.
- IC_boss: A list of information criteria (IC) for BOSS, where each element in the list is a vector representing values of a given IC for each candidate subset of BOSS (or each column in beta_boss). The output IC includes AIC, BIC, AICc, BICc, GCV and Mallows' Cp. Note that each IC is calculated by plugging in hdf_boss.

Author(s)

Sen Tian

References

- Tian, S., Hurvich, C. and Simonoff, J. (2019), On the Use of Information Criteria for Subset Selection in Least Squares Regression. https://arxiv.org/abs/1911.10191
- BOSSreg Vignette https://github.com/sentian/BOSSreg/blob/master/r-package/vignettes/BOSSreg.pdf

See Also

predict and coef methods for "boss" object, and the cv.boss function

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0 set.seed(11)

n = 20

p = 5

x = matrix(rnorm(n*p), nrow=n, ncol=p)
```

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```
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x%*%beta + scale(rnorm(n, sd=0.01), center = TRUE, scale = FALSE)
## Fit the model
boss_result = boss(x, y)
## Get the coefficient vector selected by AICc-hdf (S3 method for boss)
beta_boss_aicc = coef(boss_result)
# the above is equivalent to the following
beta_boss_aicc = boss_result$beta_boss[, which.min(boss_result$IC_boss$aicc), drop=FALSE]
## Get the fitted values of BOSS-AICc-hdf (S3 method for boss)
mu_boss_aicc = predict(boss_result, newx=x)
# the above is equivalent to the following
mu_boss_aicc = cbind(1,x) %*% beta_boss_aicc
## Repeat the above process, but using Cp-hdf instead of AICc-hdf
## coefficient vector
beta_boss_cp = coef(boss_result, method.boss='cp')
beta_boss_cp = boss_result$beta_boss[, which.min(boss_result$IC_boss$cp), drop=FALSE]
## fitted values of BOSS-Cp-hdf
mu_boss_cp = predict(boss_result, newx=x, method.boss='cp')
mu_boss_cp = cbind(1,x) %*% beta_boss_cp
```

calc.ic

Calculate an information criterion.

Description

Calculate a specified information criterion (IC) for an estimate or a group of estimates. The choices of IC include AIC, BIC, AICc, BICc, GCV and Mallows' Cp.

Usage

```
calc.ic(y_hat, y, ic = c("aicc", "bicc", "aic", "bic", "gcv", "cp"), df,
  sigma = NULL)
```

Arguments

y_hat	A vector of fitted values with length(y_hat)=length(y)=n, or a matrix, with nrow(coef)=length(y)=n and ncol(y_hat)=m, containing m different fits.
У	A vector of response variable, with length(y)=n.
ic	A specified IC to calculate. Default is AICc ('aicc'). Other choices include AIC ('aic'), BIC ('bic'), BICc ('bicc'), GCV ('gcv') and Mallows' Cp ('cp').
df	A number if y_hat is a vector, or a vector with length(df)=ncol(y_hat)=m if y_hat is a matrix. df represents the degrees of freedom for each fit.
sigma	Standard deviation of the error term. It only needs to be specified if the argument ic='cp'.

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Details

This function enables the computation of various common IC for model fits, which can further be used to choose the optimal fit. This allows user comparing the effect of different IC. In order to calculate an IC, degrees of freedoms (df) needs to be specified. To be more specific, here are the formulas used to calculate each IC:

$$AIC = \log(\frac{RSS}{n}) + 2\frac{df}{n}$$

$$BIC = \log(\frac{RSS}{n}) + \log(n)\frac{df}{n}$$

$$AICc = \log(\frac{RSS}{n}) + 2\frac{df+1}{n-df-2}$$

$$BICc = \log(\frac{RSS}{n}) + \log(n)\frac{df+1}{n-df-2}$$

$$GCV = \frac{RSS}{(n-df)^2}$$

$$Mallows'Cp = RSS + 2 \times \sigma^2 \times df$$

Value

The value(s) of the specified IC for each fit.

Author(s)

Sen Tian

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0
set.seed(11)
n = 20
p = 5
x = matrix(rnorm(n*p), nrow=n, ncol=p)
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x%*%beta + scale(rnorm(20, sd=0.01), center = TRUE, scale = FALSE)

## Fit the model
boss_result = boss(x, y)
## Print the values of AICc-hdf for all subsets given by BOSS
print(boss_result$IC_boss$aicc)
## calculate them manually using the calc.ic function
y_hat = cbind(rep(1,n),x)%*%boss_result$beta_boss
print(calc.ic(y_hat, y, df=boss_result$hdf_boss))
```

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coef.boss

Select coefficient vector(s) for BOSS.

Description

This function returns the optimal coefficient vector of BOSS selected by AICc (by default) or other types of information criterion.

Usage

```
## S3 method for class 'boss'
coef(object, ic = c("aicc", "bicc", "aic", "bic", "gcv",
   "cp"), select.boss = NULL, ...)
```

Arguments

object	The boss object, returned from calling the boss function.
ic	Which information criterion is used to select the optimal coefficient vector for BOSS. The default is AICc-hdf.
select.boss	The index (or indicies) of columns in the coefficient matrix for which one wants to select. By default (NULL) it's selected by the information criterion specified in 'ic'.
	Extra arguments (unused for now)

Details

If select.boss is specified, the function returns corresponding column(s) in the coefficient matrix.

If select.boss is unspecified, the function returns the optimal coefficient vector selected by AICc-hdf (other choice of IC can be specified in the argument ic). The only exception is when n>=p, where hdf is not well defined, and the entire coefficient matrix is returned.

Value

The chosen coefficient vector(s) for BOSS.

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0
set.seed(11)
n = 20
p = 5
x = matrix(rnorm(n*p), nrow=n, ncol=p)
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x%*%beta + scale(rnorm(n, sd=0.01), center = TRUE, scale = FALSE)
## Fit the model
boss_result = boss(x, y)
## Get the coefficient vector selected by AICc-hdf (S3 method for boss)
```

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```
beta_boss_aicc = coef(boss_result)
# the above is equivalent to the following
beta_boss_aicc = boss_result$beta_boss[, which.min(boss_result$IC_boss$aicc), drop=FALSE]
## Get the fitted values of BOSS-AICc-hdf (S3 method for boss)
mu_boss_aicc = predict(boss_result, newx=x)
# the above is equivalent to the following
mu_boss_aicc = cbind(1,x) %**% beta_boss_aicc

## Repeat the above process, but using Cp-hdf instead of AICc-hdf
## coefficient vector
beta_boss_cp = coef(boss_result, method.boss='cp')
beta_boss_cp = boss_result$beta_boss[, which.min(boss_result$IC_boss$cp), drop=FALSE]
## fitted values of BOSS-Cp-hdf
mu_boss_cp = predict(boss_result, newx=x, method.boss='cp')
mu_boss_cp = cbind(1,x) %*% beta_boss_cp
```

coef.cv.boss

Select coefficient vector based on cross-validation for BOSS or FS.

Description

This function returns coefficient vector that minimizes out-of-sample (OOS) cross validation score.

Usage

```
## S3 method for class 'cv.boss'
coef(object, method = c("boss", "fs"), ...)
```

Arguments

object The cv.boss object, returned from calling cv.boss function.

method It can either be 'fs' or 'boss'. The default is 'boss'.

Extra arguments (unused for now).

Value

The chosen coefficient vector for BOSS or FS.

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0
set.seed(11)
n = 20
p = 5
x = matrix(rnorm(n*p), nrow=n, ncol=p)
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x%*%beta + scale(rnorm(20, sd=0.01), center = TRUE, scale = FALSE)

## Perform 10-fold CV without replication
boss_cv_result = cv.boss(x, y)
## Get the coefficient vector of BOSS that gives minimum CV OSS score (S3 method for cv.boss)
```

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```
beta_boss_cv = coef(boss_cv_result)
# the above is equivalent to
boss_result = boss_cv_result$boss
beta_boss_cv = boss_result$beta_boss[, boss_cv_result$i.min.boss, drop=FALSE]
## Get the fitted values of BOSS-CV (S3 method for cv.boss)
mu_boss_cv = predict(boss_cv_result, newx=x)
# the above is equivalent to
mu_boss_cv = cbind(1,x) %*% beta_boss_cv

## Get the coefficient vector of FS that gives minimum CV OSS score (S3 method for cv.boss)
beta_fs_cv = coef(boss_cv_result, method='fs')
## Get the fitted values of FS-CV (S3 method for cv.boss)
mu_fs_cv = predict(boss_cv_result, newx=x, method='fs')
```

cv.boss

Cross-validation for Best Orthogonalized Subset Selection (BOSS) and Forward Stepwise Selection (FS).

Description

Cross-validation for Best Orthogonalized Subset Selection (BOSS) and Forward Stepwise Selection (FS).

Usage

```
cv.boss(x, y, n.folds = 10, n.rep = 1, intercept = TRUE, ...)
```

Arguments

X	A matrix of predictors, see boss.
У	A vector of response variable, see boss.
n.folds	The number of cross validation folds. Default is 10.
n.rep	The number of replications of cross validation. Default is 1.
intercept	Logical, whether to fit an intercept term. Default is TRUE.
	Arguments to boss, such as hdf.ic.boss.

Details

This function fits BOSS and FS (boss) on the full dataset, and performs n.folds cross-validation. The cross-validation process can be repeated n.rep times to evaluate the out-of-sample (OOS) performance for the candidate subsets given by both methods.

Value

- boss: An object boss that fits on the full dataset.
- n.folds: The number of cross validation folds.
- cvm.fs: Mean OOS deviance for each candidate given by FS.
- cvm.boss: Mean OSS deviance for each candidate given by BOSS.
- i.min.fs: The index of minimum cvm.fs.
- i.min.boss: The index of minimum cvm.boss.

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Author(s)

Sen Tian

References

• Tian, S., Hurvich, C. and Simonoff, J. (2019), On the Use of Information Criteria for Subset Selection in Least Squares Regression. https://arxiv.org/abs/1911.10191

• BOSSreg Vignette https://github.com/sentian/BOSSreg/blob/master/r-package/vignettes/BOSSreg.pdf

See Also

predict and coef methods for cv.boss object, and the boss function

Examples

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0
set.seed(11)
n = 20
p = 5
x = matrix(rnorm(n*p), nrow=n, ncol=p)
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x\%*beta + scale(rnorm(20, sd=0.01), center = TRUE, scale = FALSE)
## Perform 10-fold CV without replication
boss_cv_result = cv.boss(x, y)
## Get the coefficient vector of BOSS that gives minimum CV OSS score (S3 method for cv.boss)
beta_boss_cv = coef(boss_cv_result)
# the above is equivalent to
boss_result = boss_cv_result$boss
beta_boss_cv = boss_result$beta_boss[, boss_cv_result$i.min.boss, drop=FALSE]
## Get the fitted values of BOSS-CV (S3 method for cv.boss)
mu_boss_cv = predict(boss_cv_result, newx=x)
# the above is equivalent to
mu_boss_cv = cbind(1,x) %*% beta_boss_cv
## Get the coefficient vector of FS that gives minimum CV OSS score (S3 method for cv.boss)
beta_fs_cv = coef(boss_cv_result, method='fs')
## Get the fitted values of FS-CV (S3 method for cv.boss)
mu_fs_cv = predict(boss_cv_result, newx=x, method='fs')
```

predict.boss

Prediction given new data entries.

Description

This function returns the prediction(s) given new observation(s), for BOSS, where the optimal coefficient vector is chosen via certain selection rule.

Usage

```
## S3 method for class 'boss'
predict(object, newx, ...)
```

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Arguments

object The boss object, returned from calling 'boss' function.

A new data entry or several entries. It can be a vector, or a matrix with nrow(newx) being the number of new entries and ncol(newx)=p being the number of predictors. The function takes care of the intercept, NO need to add 1 to newx.

Extra arguments to be plugged into coef, such as select.boss, see the description of coef.boss for more details.

Details

The function basically calculates x * coef, where coef is a coefficient vector chosen by a selection rule. See more details about the default and available choices of the selection rule in the description of coef.boss.

Value

The prediction(s) for BOSS.

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0
set.seed(11)
n = 20
p = 5
x = matrix(rnorm(n*p), nrow=n, ncol=p)
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x%*%beta + scale(rnorm(n, sd=0.01), center = TRUE, scale = FALSE)
## Fit the model
boss_result = boss(x, y)
## Get the coefficient vector selected by AICc-hdf (S3 method for boss)
beta_boss_aicc = coef(boss_result)
# the above is equivalent to the following
beta_boss_aicc = boss_result$beta_boss[, which.min(boss_result$IC_boss$aicc), drop=FALSE]
## Get the fitted values of BOSS-AICc-hdf (S3 method for boss)
mu_boss_aicc = predict(boss_result, newx=x)
# the above is equivalent to the following
mu_boss_aicc = cbind(1,x) %*% beta_boss_aicc
## Repeat the above process, but using Cp-hdf instead of AICc-hdf
## coefficient vector
beta_boss_cp = coef(boss_result, method.boss='cp')
beta_boss_cp = boss_result$beta_boss[, which.min(boss_result$IC_boss$cp), drop=FALSE]
## fitted values of BOSS-Cp-hdf
mu_boss_cp = predict(boss_result, newx=x, method.boss='cp')
mu_boss_cp = cbind(1,x) %*% beta_boss_cp
```

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predict.cv.boss

Prediction given new data entries.

Description

This function returns the prediction(s) given new observation(s) for BOSS or FS, where the optimal coefficient vector is chosen via cross-validation.

Usage

```
## S3 method for class 'cv.boss'
predict(object, newx, ...)
```

Arguments

object The cv.boss object, returned from calling cv.boss function.

newx A new data entry or several entries. It can be a vector, or a matrix with nrow(newx)

being the number of new entries and ncol(newx)=p being the number of predictors. The function takes care of the intercept, NO need to add 1 to newx.

Extra arguments to be plugged into coef, such as method, see the description of

coef.cv.boss for more details.

Value

The prediction for BOSS or FS.

```
## Generate a trivial dataset, X has mean 0 and norm 1, y has mean 0 \,
set.seed(11)
n = 20
p = 5
x = matrix(rnorm(n*p), nrow=n, ncol=p)
x = scale(x, center = colMeans(x))
x = scale(x, scale = sqrt(colSums(x^2)))
beta = c(1, 1, 0, 0, 0)
y = x%*%beta + scale(rnorm(20, sd=0.01), center = TRUE, scale = FALSE)
## Perform 10-fold CV without replication
boss_cv_result = cv.boss(x, y)
## Get the coefficient vector of BOSS that gives minimum CV OSS score (S3 method for cv.boss)
beta_boss_cv = coef(boss_cv_result)
# the above is equivalent to
boss_result = boss_cv_result$boss
beta_boss_cv = boss_result$beta_boss[, boss_cv_result$i.min.boss, drop=FALSE]
## Get the fitted values of BOSS-CV (S3 method for cv.boss)
mu_boss_cv = predict(boss_cv_result, newx=x)
# the above is equivalent to
mu_boss_cv = cbind(1,x) %*% beta_boss_cv
## Get the coefficient vector of FS that gives minimum CV OSS score (S3 method for cv.boss)
beta_fs_cv = coef(boss_cv_result, method='fs')
## Get the fitted values of FS-CV (S3 method for cv.boss)
mu_fs_cv = predict(boss_cv_result, newx=x, method='fs')
```

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