Package ‘pcLasso’

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Author Jerome Friedman, Kenneth Tay, Robert Tibshirani
Maintainer Rob Tibshirani <tibs@stanford.edu>
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Cross-validation for pcLasso

Description

Does k-fold cross-validation for pcLasso.

Usage

cv.pcLasso(x, y, w = rep(1, length(y)), ratio = NULL, theta = NULL,
groups = vector("list", 1), family = "gaussian", nfolds = 10,
foldid = NULL, keep = FALSE, verbose = FALSE, ...)

Arguments

x x matrix as in pcLasso.
y y matrix as in pcLasso.
w Observation weights. Default is 1 for each observation.
ratio Ratio of shrinkage between the second and first principal components in the absence of the $\ell_1$ penalty. More convenient way to specify the strength of the quadratic penalty. A value between 0 and 1 (only 1 included). ratio = 1 corresponds to the lasso, 0.5-0.9 are good values to use. Default is NULL. Exactly one of ratio or theta must be specified.
theta Multiplier for the quadratic penalty: a non-negative real number. theta = 0 corresponds to the lasso, and larger theta gives strong shrinkage toward the top principal components. Default is NULL. Exactly one of ratio or theta must be specified.
groups A list describing which features belong in each group. The length of the list should be equal to the number of groups, with groups[[k]] being a vector of feature/column numbers which belong to group k. Each feature must be assigned to at least one group. Features can belong to more than one group. By default, all the features belong to a single group.
family Response type. Either "gaussian" (default) for linear regression or "binomial" for logistic regression.
nfolds Number of folds for CV (default is 10). Although nfolds can be as large as the sample size (leave-one-out CV), it is not recommended for large datasets. Smallest value allowable is nfolds = 3.
foldid An optional vector of values between 1 and nfold identifying what fold each observation is in. If supplied, nfold can be missing.
keep If keep = TRUE, a prevalidated array is returned containing fitted values for each observation at each value of lambda. This means these fits are computed with this observation and the rest of its fold omitted. Default is FALSE.
verbose Print out progress along the way? Default is FALSE.
... Other arguments that can be passed to pcLasso.
cv.pclasso

Details

This function runs pclasso nfolds+1 times: the first to get the lambda sequence, and the remaining nfolds times to compute the fit with each of the folds omitted. The error is accumulated, and the mean error and standard deviation over the folds is computed. Note that cv.pclasso does NOT search for values of theta or ratio. A specific value of theta or ratio should be supplied.

Value

An object of class "cv.pclasso", which is a list with the ingredients of the cross-validation fit.

- glmfit: A fitted pclasso object for the full data.
- theta: Value of theta used in model fitting.
- lambda: The values of lambda used in the fits.
- nzero: If the groups overlap, the number of non-zero coefficients in the model glmfit for the expanded feature space, at each value of lambda. Otherwise, the number of non-zero coefficients in the model glmfit for the original feature space.
- originzero: If the groups are overlapping, this is the number of non-zero coefficients in the model glmfit for the original feature space, at each lambda. If groups are not overlapping, it is NULL.
- fit.preval: If keep=TRUE, this is the array of prevalidated fits.
- cvm: The mean cross-validated error: a vector of length length(lambda).
- cvse: Estimate of standard error of cvm.
- cvlo: Lower curve = cvm - cvsd.
- cvup: Upper curve = cvm + cvsd.
- lambda.min: The value of lambda that gives minimum cvm.
- lambda.1se: The largest value of lambda such that the CV error is within one standard error of the minimum.
- foldid: If keep=TRUE, the fold assignments used.
- name: Name of error measurement used for CV.
- call: The call that produced this object.

See Also

pclasso and plot.cv.pclasso.

Examples

set.seed(1)
x <- matrix(rnorm(100 * 20), 100, 20)
y <- rnorm(100)
groups <- vector("list", 4)
for (k in 1:4) {
  groups[[k]] <- 5 * (k-1) + 1:5
}
svfit1 <- cv.pclasso(x, y, groups = groups, ratio = 0.8)
pcLasso

Fit a model with principal components lasso

Description

Fit a model using the principal components lasso for an entire regularization path indexed by the parameter lambda. Fits linear and logistic regression models.

Usage

```
pclasso(x, y, w = rep(1, length(y)), family = c("gaussian", "binomial"), ratio = NULL, theta = NULL, groups = vector("list", 1), lambda.min.ratio = ifelse(nrow(x) < ncol(x), 0.01, 1e-04), nlam = 100, lambda = NULL, standardize = F, svd_info = NULL, nv = NULL, propack = T, thr = 1e-04, maxit = 1e+05, verbose = FALSE)
```

Arguments

- **x**: Input matrix, of dimension nobs x nvars; each row is an observation vector.
- **y**: Response variable. Quantitative for family = "gaussian". For family="binomial", should be a numeric vector consisting of 0s and 1s.
- **w**: Observation weights. Default is 1 for each observation.
- **family**: Response type. Either "gaussian" (default) for linear regression or "binomial" for logistic regression.
- **ratio**: Ratio of shrinkage between the second and first principal components in the absence of the ℓ_1 penalty. More convenient way to specify the strength of the quadratic penalty. A value between 0 and 1 (only 1 included). ratio = 1 corresponds to the lasso, 0.5-0.9 are good values to use. Default is NULL. Exactly one of ratio or theta must be specified.
- **theta**: Multiplier for the quadratic penalty: a non-negative real number. theta = 0 corresponds to the lasso, and larger theta gives strong shrinkage toward the top principal components. Default is NULL. Exactly one of ratio or theta must be specified.
A list describing which features belong in each group. The length of the list should be equal to the number of groups, with \texttt{groups[[k]]} being a vector of feature/column numbers which belong to group \(k\). Each feature must be assigned to at least one group. Features can belong to more than one group. By default, all the features belong to a single group.

**lambda.min.ratio**

Smallest value for \(\lambda\), as a fraction of the largest \(\lambda\) value. The default depends on the sample size \(nobs\) relative to the number of variables \(nvars\). If \(nobs \geq nvars\), the default is 0.0001, close to zero. If \(nobs < nvars\), the default is 0.01. This is only used when the user does not specify a \(\lambda\) sequence.

**nlam**

Number of \(\lambda\) values; default is 100.

**lambda**

A user supplied \(\lambda\) sequence. Typical usage is to have the program compute its own \(\lambda\) sequence based on \texttt{nlam} and \texttt{lambda.min.ratio}; supplying a value of \(\lambda\) overrides this.

**standardize**

If \texttt{TRUE}, the columns of the feature matrices are standardized before the algorithm is run. Default is \texttt{FALSE}.

**SVD.info**

A list containing SVD information. Usually this should not be specified by the user: the function will compute it on its own by default. \texttt{SVD.info} is a list with three elements:

1. \(aa\): A row-wise concatenation of the \(k\) quadratic penalty matrices.
2. \(d\): A list where the \(k\)th element is the vector of squared singular values of the input matrix corresponding to group \(k\).
3. \(dd\): A list where the \(k\)th element is the vector of \(d_{k1}^2 - d_{kj}^2\) for the input matrix corresponding to group \(k\).

Since the initial SVD of \(x\) can be the largest part of the overall computation, we allow the user to compute it once and then re-use. See example below.

**nv**

Number of singular vectors to use in the singular value decompositions. If not specified, the full SVD is used.

**propack**

If \texttt{TRUE} (default), uses \texttt{propack.svd} from the \texttt{svd} package to perform the singular value decompositions. If not, uses \texttt{svd} from base R.

**thr**

Convergence threshold for the coordinate descent algorithm. Default is \(1e^{-4}\).

**maxit**

Maximum number of passes over the data for all \(\lambda\) values; default is \(1e5\).

**verbose**

Print out progress along the way? Default is \texttt{FALSE}.

### Details

The objective function for "gaussian" is

\[
1/2 \text{RSS}/nobs + \lambda \cdot ||\beta||_1 + \theta/2 \sum \text{quadraticpenalty for group } k,
\]

where the sum is over the feature groups \(1, \ldots, K\). The objective function for "binomial" is

\[
-\loglik/nobs + \lambda \cdot ||\beta||_1 + \theta/2 \sum \text{quadraticpenalty for group } k.
\]
pcLasso can handle overlapping groups. In this case, the original \( x \) matrix is expanded to a \( nobs \times p_{1\ldots K} \) matrix (where \( p_k \) is the number of features in group \( k \)) such that columns \( p_{1\ldots k-1} + 1 \) to \( p_{1\ldots K} \) represent the feature matrix for group \( k \). pcLasso returns the model coefficients for both the expanded feature space and the original feature space.

One needs to specify the strength of the quadratic penalty either by specifying ratio, which is the ratio of shrinkage between the second and first principal components in the absence of the \( \ell_1 \) penalty, or by specifying the multiplier theta. ratio is unitless and is more convenient.

pcLasso always mean centers the columns of the \( x \) matrix. If standardize=TRUE, pcLasso will also scale the columns to have standard deviation 1. In all cases, the beta coefficients returned are for the original \( x \) values (i.e. uncentered and unscaled).

**Value**

An object of class "pcLasso".

- **beta**: If the groups overlap, a \( p_{1\ldots K} \times \text{length}(\lambda) \) matrix of coefficients in the expanded feature space. If not, a \( nvars \times \text{length}(\lambda) \) matrix of coefficients in the original feature space.
- **origbeta**: If the groups overlap, a \( nvars \times \text{length}(\lambda) \) matrix of coefficients in the original feature space. NULL if the groups do not overlap.
- **a0**: Intercept sequence of length \( \text{length}(\lambda) \).
- **lambda**: The actual sequence of \( \lambda \) values used.
- **nzero**: If the groups overlap, the number of non-zero coefficients in the expanded feature space for each value of \( \lambda \). Otherwise, the number of non-zero coefficients in the original feature space.
- **orignzero**: If the groups are overlapping, this is the number of non-zero coefficients in the original feature space of the model for each \( \lambda \). If groups are not overlapping, it is NULL.
- **jerr**: Error flag for warnings and errors (largely for internal debugging).
- **theta**: Value of theta used in model fitting.
- **origgroups**: If the groups parameter was passed to the function call, this is a copy of that parameter. Otherwise, it is a list of length 1, with the first element being a vector of integers from 1 to \( nvars \).
- **groups**: If the groups are not overlapping, this has the same value as groups. If the groups are overlapping, then \( \text{groups}[[k]] \) is the vector from \( p_{1\ldots k-1} + 1 \) to \( p_k \), where \( p_k \) is the number of features in group \( k \).
- **SVD_info**: A list containing SVD information. See param SVD_info for more information.
- **mx**: If groups overlap, column means of the expanded \( x \) matrix. Otherwise, column means of the original \( x \) matrix.
- **origmx**: Column means of the original \( x \) matrix.
- **my**: If family = "gaussian", mean of the responses \( y \). Otherwise, it is NA.
- **overlap**: A logical flag indicating if the feature groups were overlapping or not.
- **nlp**: Actual number of passes over the data for all \( \lambda \) values.
- **family**: Response type.
- **call**: The call that produced this object.
**Examples**

```r
set.seed(1)
x <- matrix(rnorm(100 * 20), 100, 20)
y <- rnorm(100)

# all features in one group by default
fit1 <- plasso(x, y, ratio = 0.8)
# print(fit1) # Not run
# features in groups
groups <- vector("list", 4)
for (k in 1:4) {
  groups[[k]] <- 5 * (k-1) + 1:5
}
fit2 <- plasso(x, y, groups = groups, ratio = 0.8)
# groups can be overlapping
groups[[1]] <- 1:8
fit3 <- plasso(x, y, groups = groups, ratio = 0.8)

# specify ratio or theta, but not both
fit4 <- plasso(x, y, groups = groups, theta = 10)

# family = "binomial"
y2 <- sample(0:1, 100, replace = TRUE)
fit5 <- plasso(x, y2, ratio = 0.8, family = "binomial")

# example where SVD is computed once, then re-used
fit1 <- plasso(x, y, ratio = 0.8)
fit2 <- plasso(x, y, ratio = 0.8, SVD_info = fit1$SVD_info)
```

---

**plot.cv.pclasso**  
*Plot the cross-validation curve produced by "cv.pclasso" object*

**Description**

Plots the cross-validation curve produced by a cv.pclasso object, along with upper and lower standard deviation curves, as a function of the lambda values used.

**Usage**

```r
## S3 method for class 'cv.pclasso'
plot(x, sign.lambda = 1, originz = TRUE, ...)
```

**Arguments**

- `x` Fitted "cv.pclasso" object.
- `sign.lambda` Either plot against log(lambda) (default) or -log(lambda) (if sign.lambda = -1).
predict.cv.pcLasso

originz

If TRUE (default), prints the number of non-zero coefficients in the original feature space. If not, prints the number of non-zero coefficients in the expanded feature space. No effect if groups are not overlapping.

Other graphical parameters to plot.

Details

A plot is produced and nothing is returned.

See Also

pclasso and cv.pclasso.

Examples

set.seed(1)
x <- matrix(rnorm(100 * 20), 100, 20)
y <- rnorm(100)
groups <- vector("list", 4)
for (k in 1:4) {
  groups[[k]] <- 5 * (k-1) + 1:5
}
cvfit <- cv.pclasso(x, y, ratio = 0.8, groups = groups)
plot(cvfit)
# plot flipped: x-axis tracks -log(lambda) instead
plot(cvfit, sign.lambda = -1)

# if groups overlap, originz can be used to decide which space to count the
# number of non-zero coefficients at the top

groups[[1]] <- 1:8
cvfit <- cv.pclasso(x, y, ratio = 0.8, groups = groups)
plot(cvfit)  # no. of non-zero coefficients in original space
plot(cvfit, originz = FALSE)  # no. of non-zero coefficients in expanded space

predict.cv.pclasso  

Make predictions from a "cv.pclasso" object

Description

This function returns the predictions for a new data matrix from a cross-validated pcLasso model by using the stored "glmfit" object and the optimal value chosen for lambda.

Usage

## S3 method for class 'cv.pclasso'
predict(object, xnew, s = c("lambda.1se", "lambda.min"), ...)
predict.pcLasso

Arguments

- object: Fitted "cv.pcLasso" object.
- xnew: Matrix of new values for x at which predictions are to be made.
- s: Value of the penalty parameter lambda at which predictions are required. Default is the value s="lambda.1se" stored in the CV fit. Alternatively, s="lambda.min" can be used.
- ...: Potentially other arguments to be passed to and from methods; currently not in use.

Details

This function makes it easier to use the results of cross-validation to make a prediction. Note that xnew should have the same number of columns as the original feature space, regardless of whether the groups are overlapping or not.

Value

Predictions which the cross-validated model makes for xnew at the optimal value of lambda. Note that the default is the "lambda.1se" for lambda, to make this function consistent with cv.glmnet in the glmnet package. The output is predictions of $E(y|x_{new})$: these are probabilities for the binomial family.

See Also

cv.pcLasso and predict.pcLasso.

Examples

```r
set.seed(1)
x <- matrix(rnorm(100 * 20), 100, 20)
y <- rnorm(100)
cvfit <- cv.pclasso(x, y, ratio = 0.8)
predict(cvfit, xnew = x[1:5, ])
predict(cvfit, xnew = x[1:5, ], s = "lambda.min")
```

---

```
predict.pcLasso

Make predictions from a "pcLasso" object

Description

This function returns the predictions from a "pcLasso" object for a new data matrix.

Usage

```r
## S3 method for class 'pcLasso'
predict(object, xnew, ...)
```
Arguments

- **object**: Fitted "pcLasso" object.
- **xnew**: Matrix of new values for \( x \) at which predictions are to be made.
- **...**: Potentially other arguments to be passed to and from methods; currently not in use.

Details

Note that \( x_{\text{new}} \) should have the same number of columns as the original feature space, regardless of whether the groups are overlapping or not.

Value

Predictions of \( E(y|x_{\text{new}}) \) which the model \texttt{object} makes at \( x_{\text{new}} \). These are probabilities for the binomial family.

See Also

\texttt{pcLasso}.

Examples

```r
set.seed(1)
x <- matrix(rnorm(100 * 20), 100, 20)

# family = "gaussian"
y <- rnorm(100)
fit1 <- pcLasso(x, y, ratio = 0.8)
predict(fit1, xnew = x[1:5, ])

# family = "binomial"
y2 <- sample(0:1, 100, replace = TRUE)
fit2 <- pcLasso(x, y2, ratio = 0.8, family = "binomial")
predict(fit2, xnew = x[1:5, ])
```
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