

Package ‘parcor’

February 15, 2012

Type Package

Title Regularized estimation of partial correlation matrices

Version 0.2-2

Date 2010-01-05

Depends MASS, glmnet, ppls, Epi, GeneNet

Author Nicole Kraemer, Juliane Schaefer

Maintainer Nicole Kraemer <nkraemer@cs.tu-berlin.de>

Description The package estimates the matrix of partial correlations based on different regularized regression methods: lasso, adaptive lasso, PLS, and Ridge Regression. In addition, the package provides model selection for lasso, adaptive lasso and Ridge regression based on cross-validation.

License GPL (>= 2)

LazyLoad yes

Repository CRAN

Date/Publication 2010-01-06 12:11:55

R topics documented:

parcor-package	2
adalasso	2
adalasso.net	4
Beta2parcor	5
mylars	7
performance.pcor	8
pls.net	9
ridge.cv	10
ridge.net	11
sym2vec	12

Index	14
--------------	-----------

parcor-package	<i>Parcor: Estimation of partial correlations based on regularized regression.</i>
----------------	--

Description

This package contains different methods to estimate the matrix of partial correlations based on a $(n \times p)$ matrix X of observation. For low-dimensional settings ($p > n$), the matrix of partial correlations can be estimated based on p least-squares regression fits. However, in high-dimensional scenarios ($p < n$), these least-squares problems are ill-posed and need to be regularized. This package contains four different regularized regression techniques for the estimation of the partial correlations: lasso, adaptive lasso, ridge regression, and Partial Least Squares. In addition, the package provides model selection for lasso, adaptive lasso and Ridge regression based on cross-validation.

Details

Package:	parcor
Type:	Package
Version:	0.2-1
Date:	2009-11-17
License:	GPL2 or newer
LazyLoad:	yes

Author(s)

Nicole Kraemer, Juliane Schaefer
Maintainer: Nicole Kraemer <nkraemer@cs.tu-berlin.de>

References

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks with Gaussian Graphical Models", BMC Bioinformatics, 10:384
<http://www.biomedcentral.com/1471-2105/10/384/>

adalasso	<i>Adaptive Lasso</i>
----------	-----------------------

Description

This function computes the lasso and adaptive lasso solution based on k -fold cross-validation. The initial weights for adaptive lasso are computed from a lasso fit.

Usage

```
adalamo(X, y, k = 10, use.Gram = TRUE, both=TRUE)
```

Arguments

X	matrix of input observations. The rows of X contain the samples, the columns of X contain the observed variables
y	vector of responses. The length of y must equal the number of rows of X
k	the number of splits in k-fold cross-validation. The same k is used for the estimation of the weights and the estimation of the penalty term for adaptive lasso. Default is k=10.
use.Gram	When the number of variables is very large, you may not want LARS to pre-compute the Gram matrix. Default is use.Gram=TRUE.
both	Logical. If both=FALSE, only the lasso coefficients are computed. Default is both=TRUE.

Details

In each of the k-fold cross-validation steps, the weights for adaptive lasso are computed in terms of a lasso fit. (The optimal value of the penalty term is selected via k-fold cross-validation). Note that this implies that a lasso solution is computed $k*k$ times!

Value

intercept.lasso	intercept for lasso.
intercept.adalamo	intercept for adaptive lasso.
coefficients.adalamo	regression coefficients for adaptive lasso.
coefficients.lasso	regression coefficients for lasso.
cv.lasso	cv error for the optimal lasso model.
cv.adalamo	cv error for the optimal adaptive lasso model.
lambda.lasso	optimal lambda value for lasso-
lambda.adalamo	optimal lambda value for adaptive lasso.

Author(s)

Nicole Kraemer, Juliane Schaefer

References

H. Zou (2006) "The Adaptive Lasso and its Oracle Property", Journal of the American Statistical Association 101 (476): 1418-1429.

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks using Gaussian Graphical Models", BMC Bioinformatics, 10:384

<http://www.biomedcentral.com/1471-2105/10/384/>

See Also

[Beta2parcor](#), [adalasso.net](#)

Examples

```
n<-100 # number of observations
p<-60 # number of variables
X<-matrix(rnorm(n*p),ncol=p)
y<-rnorm(n)
ada.object<-adalasso(X,y,k=10)
```

adalasso.net

Partial Correlations with (Adaptive) Lasso

Description

This function computes the matrix of partial correlations based on an estimation of the corresponding regression models via lasso and adaptive lasso respectively.

Usage

```
adalasso.net(X, k = 10, use.Gram=FALSE, both=TRUE, verbose=FALSE)
```

Arguments

X	matrix of observations. The rows of X contain the samples, the columns of X contain the observed variables.
k	the number of splits in k-fold cross-validation. The same k is used for the estimation of the weights and the estimation of the penalty term for adaptive lasso. Default value is k=10.
use.Gram	When the number of variables is very large, you may not want LARS to pre-compute the Gram matrix. Default is use.Gram=FALSE.
both	Logical. If both=FALSE, only the lasso solution is computed. Default is both=TRUE.
verbose	Print information on conflicting signs etc. Default is verbose=FALSE

Details

For each of the columns of X , a regression model based on (adaptive) lasso is computed. In each of the k -fold cross-validation steps, the weights for adaptive lasso are computed in terms of a lasso fit. (The optimal value of the penalty term is selected via k -fold cross-validation). Note that this implies that a lasso solution is computed $k*k$ times! Finally, the results of the regression models are transformed via the function Beta2parcor.

Value

pcor.adalasso estimated matrix of partial correlation coefficients for adaptive lasso.
pcor.lasso estimated matrix of partial correlation coefficients for lasso.
...

Author(s)

Nicole Kraemer

References

H. Zou (2006) "The Adaptive Lasso and its Oracle Property", Journal of the American Statistical Association. 101 (476): 1418-1429.

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks using Gaussian Graphical Models", BMC Bioinformatics, 10:384

<http://www.biomedcentral.com/1471-2105/10/384/>

See Also

[Beta2parcor](#), [adalasso](#)

Examples

```
n<-20
p<-10
X<-matrix(rnorm(n*p),ncol=p)
pc<-adalasso.net(X,k=5)
```

Beta2parcor

Computation of partial correlation coefficients

Description

This function computes the matrix of partial correlation coefficients based on the results of the corresponding regression models.

Usage

```
Beta2parcor(Beta, verbose=FALSE)
```

Arguments

Beta	matrix of regression coefficients
verbose	print information on conflicting signs etc. Default is verbose=FALSE.

Details

A well-known result (Whittaker, 1990) shows that the matrix of partial correlation coefficients can be estimated by computing a least squares regression model for each variable. If there are more variables than observations, the least squares problem is ill-posed and needs regularization. The matrix Beta stores the regression coefficients of any user-defined regression method. The function Beta2parcor computes the corresponding matrix of partial correlations.

Value

matrix of partial correlation coefficients

Note

This is an internal function.

Author(s)

Nicole Kraemer

References

J. Whittaker (1990) "Graphical models in applied multivariate statistics", Wiley, New York.

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks with Gaussian Graphical Models", BMC Bioinformatics, 10:384

<http://www.biomedcentral.com/1471-2105/10/384/>

See Also

[ridge.net](#), [adalasso.net](#), [pls.net](#)

Examples

```
# this is an internal function and should not be called by the user
```

mylars *Cross-validation for Lasso*

Description

This function computes the cross-validation-optimal regression coefficients for lasso.

Usage

```
mylars(X, y, k = 10, use.Gram=TRUE, normalize=TRUE)
```

Arguments

X	matrix of observations. The rows of X contain the samples, the columns of X contain the observed variables
y	vector of responses. The length of y must equal the number of rows of X
k	the number of splits in k-fold cross-validation. Default is k=10.
use.Gram	When the number of variables is very large, you may not want LARS to pre-compute the Gram matrix. Default is use.Gram=TRUE.
normalize	Should the columns of X be scaled? Default is normalize=TRUE.

Details

We use the `glmnet()` function from the `glmnet` package to compute the fit. Note that in Kraemer et. al. (2009), we used the `lars()` function from the `lars` package, which is much slower than `glmnet()`.

Value

lambda	vector of parameter values from which the optimal parameter is selected
cv	cross-validated error for all lambda values
lambda.opt	cross-validation optimal parameter
cv.lasso	cv error for the optimal model.
intercept	cross-validation optimal intercept
coefficients	cross-validation optimal regression coefficients, without intercept

Author(s)

Nicole Kraemer

References

R. Tibshirani (1997) "Regression Shrinkage and Selection via the Lasso", *Journal of the Royal Statistical Society B*, 58 (1)

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks with Gaussian Graphical Models", *BMC Bioinformatics*, 10:384

<http://www.biomedcentral.com/1471-2105/10/384/>

See Also

[Beta2parcor](#), [adalasso](#)

Examples

```
n<-20
p<-50
X<-matrix(rnorm(n*p),ncol=p)
y<-rnorm(n)
dummy<-mylars(X,y)
```

performance.pcor

Quality of estimated partial correlations

Description

This function computed various performance measures of the estimated matrix of partial correlations.

Usage

```
performance.pcor(inferred.pcor, true.pcor=NULL, fdr=TRUE, cutoff.ggm=0.8, verbose=FALSE, plot.it=FALSE)
```

Arguments

<code>inferred.pcor</code>	matrix of estimated partial correlations
<code>true.pcor</code>	true matrix of partial correlations. Default is <code>true.pcor=NULL</code>
<code>fdr</code>	logical. If <code>fdr=TRUE</code> , the entries of <code>inferred.pcor</code> are tested for significance. Default is <code>fdr=TRUE</code>
<code>cutoff.ggm</code>	default cutoff for significant partial correlations. Default is <code>cutoff.ggm=0.8</code>
<code>verbose</code>	Print information on test results etc.. Default is <code>verbose=FALSE</code>
<code>plot.it</code>	Plot test results and ROC-curves. Default is <code>plot.it=FALSE</code>

Details

This function computes a range of performance measures: The function always returns the number of selected edges, the binary matrix that encodes the edges, the connectivity and the percentage of positive correlations. If `true.pcor` is provided, the function also returns the power (= true positive rate), the false positive rate and the positive predictive value. For non-sparse estimates that involve testing (i.e. `fdr=TRUE`) the function also returns the area under the curve, and a pair of vectors of false and true positive rates. The latter can e.g. be used to plot a ROC-curve.

Value

num.selected	number of selected edges
adj	binary matrix that encodes the existence of an edge between two nodes.
connectivity	vector of length ncol(inferred.pcor). Its ith entry indicated the number of nodes that are connected to the ith node.
positive.cor	percentage of positive partial correlations out of all selected edges.
power	power (if true.pcor is provided)
ppv	positive predictive value (if true.pcor is provided)
tpr	true positive rate (=power) (if true.pcor is provided)
fpr	true positive rate (=power) (if true.pcor is provided)
auc	area under the curve (if true.pcor is provided and fdr=TRUE)
TPR	vector of true positive rates corresponding to varying cut-offs (if true.pcor is provided and fdr=TRUE)
FPR	vector of false positive rates corresponding to varying cut-offs (if true.pcor is provided and fdr=TRUE)

Author(s)

Juliane Schaefer, Nicole Kraemer

References

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks using Gaussian Graphical Models", BMC Bioinformatics, 10:384
<http://www.biomedcentral.com/1471-2105/10/384/>

pls.net

Partial Correlations with Partial Least Squares

Description

This function computes the matrix of partial correlations via an estimation of the corresponding regression models via Partial Least Squares.

Usage

```
pls.net(X, scale = TRUE, k = 10, ncomp = 15, verbose=FALSE)
```

Arguments

X	matrix of observations. The rows of X contain the samples, the columns of X contain the observed variables.
scale	Scale the columns of X? Default is scale=TRUE.
k	Number of splits in k-fold cross-validation. Default value is k=10.
ncomp	Maximal number of components. Default is 15.
verbose	Print information on conflicting signs etc. Default is verbose=FALSE

Details

For each of the columns of X , a regression model based on Partial Least Squares is computed. The optimal model is determined via cross-validation. The results of the regression models are transformed via the function `Beta2parcor`.

Value

`pcor` estimated matrix of partial correlation coefficients.
`m` optimal number of components for each of the `ncol(X)` regression models.

Author(s)

Nicole Kraemer

References

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks using Gaussian Graphical Models", BMC Bioinformatics, 10:384
<http://www.biomedcentral.com/1471-2105/10/384/>

Examples

```
n<-20
p<-40
X<-matrix(rnorm(n*p),ncol=p)
pc<-pls.net(X,ncomp=10,k=5)
```

ridge.cv

Ridge Regression.

Description

This function computes the optimal ridge regression model based on cross-validation.

Usage

```
ridge.cv(X, y, lambda, scale = TRUE, k = 10, plot.it = FALSE)
```

Arguments

`X` matrix of input observations. The rows of X contain the samples, the columns of X contain the observed variables
`y` vector of responses. The length of y must equal the number of rows of X
`lambda` Vector of penalty terms.
`scale` Scale the columns of X ? Default is `scale=TRUE`.
`k` Number of splits in k -fold cross-validation. Default value is `k=10`.
`plot.it` Plot the cross-validation error as a function of `lambda`? Default is `FALSE`.

Value

intercept	cross-validation optimal intercept
coefficients	cross-validation optimal regression coefficients
lambda.opt	optimal value of lambda.

Author(s)

Nicole Kraemer

See Also

[ridge.net](#)

Examples

```
n<-100 # number of observations
p<-60 # number of variables
X<-matrix(rnorm(n*p),ncol=p)
y<-rnorm(n)
ridge.object<-ridge.cv(X,y)
```

ridge.net

Partial correlations with ridge regression.

Description

This function computes the matrix of partial correlations via an estimation of the corresponding regression models via Ridge Regression.

Usage

```
ridge.net(X, lambda, plot.it = FALSE, scale = TRUE, k = 10,verbose=FALSE)
```

Arguments

X	matrix of observations. The rows of X contain the samples, the columns of X contain the observed variables.
lambda	Vector of penalty terms.
scale	Scale the columns of X? Default is scale=TRUE.
k	Number of splits in k-fold cross-validation. Default value is k=10.
plot.it	Plot the cross-validation error as a function of lambda? Default is FALSE.
verbose	Print information on conflicting signs etc. Default is verbose=FALSE

Value

pcor estimated matrix of partial correlations.
lambda.opt optimal value of lambda for each of the ncol regression models.

Author(s)

Nicole Kraemer

References

N. Kraemer, J. Schaefer, A.-L. Boulesteix (2009) "Regularized Estimation of Large-Scale Gene Regulatory Networks using Gaussian Graphical Models", BMC Bioinformatics, 10:384
<http://www.biomedcentral.com/1471-2105/10/384/>

See Also

[ridge.cv](#)

Examples

```
n<-20  
p<-40  
X<-matrix(rnorm(n*p),ncol=p)  
pc<-ridge.net(X,k=5)
```

sym2vec

Transform symmetric matrix to vector

Description

This function transforms the upper triangle (without diagonal) of a matrix A into a vector.

Usage

```
sym2vec(A)
```

Arguments

A quadratic matrix of size p x p

Details

The entries of the matrix A are stacked line-by-line.

Value

vector of length $p(p-1)/2$

Note

This is an internal function.

Author(s)

Nicole Kraemer

Examples

```
p<-7  
A<-matrix(rnorm(p*p),ncol=p)  
v<-sym2vec(A)
```

Index

*Topic **multivariate**

- adalasso, [2](#)
- adalasso.net, [4](#)
- Beta2parcor, [5](#)
- mylars, [7](#)
- performance.pcor, [8](#)
- pls.net, [9](#)
- ridge.cv, [10](#)
- ridge.net, [11](#)
- sym2vec, [12](#)

*Topic **package**

- parcor-package, [2](#)

adalasso, [2](#), [5](#), [8](#)

adalasso.net, [4](#), [4](#), [6](#)

Beta2parcor, [4](#), [5](#), [5](#), [8](#)

mylars, [7](#)

parcor (parcor-package), [2](#)

parcor-package, [2](#)

performance.pcor, [8](#)

pls.net, [6](#), [9](#)

ridge.cv, [10](#), [12](#)

ridge.net, [6](#), [11](#), [11](#)

sym2vec, [12](#)