# Matlab Package: Envelope

# April 8, 2012

# Contents

Ι	Tools	4
1	$bstrp\_OLS$	4
2	center	5
3	Contr	6
4	Expan	7
5	$\operatorname{fit}_{-}\operatorname{OLS}$	8
6	WInit	9
7	Kpd	10
8	Lmatrix	11
9	$make\_parameter$	12
II	env	14
10	aic_env	14
11	bic_env	15
<b>12</b>	$2  \mathrm{bstrp\_env}$	16
13	m 6 dF4env	17
14	env	18
<b>15</b>	F4env	20

16 lrt_env	21
III henv	22
17 aic_henv	22
18 bic_henv	23
19 bstrp_henv	24
$20~\mathrm{dF4henv}$	25
21 F4henv	26
22 henv	27
23 lrt_henv	30
IV ienv	31
24 aic_ienv	31
25 bic_ienv	32
26 bstrp_ienv	33
27 dF4ienv	34
28 F4ienv	35
29 ienv	36
30 lrt_ienv	38
V penv	38
31 aic_penv	39
32 bic_penv	41
33 bstrp_penv	42
$34  \mathrm{lrt\_penv}$	44
35 penv	46

VI senv	49
36 aic_senv	49
37 bic_senv	50
$38 \text{ bstrp\_senv}$	51
39  dF4senv	52
40 F4senv	53
41 objfun	54
42 senv	55

# Part I

# Tools

# 1 bstrp\_OLS

Compute bootstrap standard error for ordinary least squares.

#### Contents

- Usage
- Description

# Usage

 $bootse=bstrp\_OLS(X,Y,B)$ 

#### Input

- X: Predictors, an n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables
- B: Number of boostrap samples. A positive integer.

#### Output

 $\bullet$  bootse: The standard error for elements in  $\beta$  computed by bootstrap. An r by p matrix.

## Description

This function computes the bootstrap standard errors for the regression coefficients in ordinary least squares by bootstrapping the residuals.

# 2 center

Substract the mean of each column

## Contents

- Usage
- Description
- $\bullet$  Example

# Usage

```
XC = center(X)
```

Input

• X: A matrix or a column vector.

Output

 $\bullet\,$  XC: A matrix or a column vector with the mean for each column equal to 0.

# Description

This function centerizes a matrix or a vector, by substracting each column by its column mean.

# Example

```
a = [1\ 2\ 3;\ 4\ 5\ 6];
```

center(a)

# 3 Contr

Compute the contraction matrix of dimension r.

#### Contents

- Usage
- Description

# Usage

C = Contr(r)

Input

• r: Dimension of the contraction matrix. A positive integer.

Output

• C: Contraction matrix of dimension r. C is an r(r+1)/2 by  $r^2$  matrix.

# Description

The contraction and expansion matrices are links between the "vec" operator and "vech" operator: for an r by r symmetric matrix A,  $\operatorname{vech}(A) = \operatorname{Contr}(r)\operatorname{vec}(A)$ , and  $\operatorname{vec}(A) = \operatorname{Expan}(r)\operatorname{vech}(A)$ . The "vec" operator stacks the matrix A into an r^2 by 1 vector columnwise. The "vech" operator stacks the lower triangle or the upper triangle of a symmetric matrix into an r(r+1)/2 vector. For more details of "vec", "vech", contraction and expansion matrix, refer to Henderson and Searle (1979).

# 4 Expan

Compute the expansion matrix of dimension r.

#### Contents

- Usage
- Description

# Usage

E = Expan(r)

Input

• r: Dimension of the expansion matrix. A positive integer.

Output

• E: Expansion matrix of dimension r. E is an  $r^2$  by r(r+1)/2 matrix.

# Description

The contraction and expansion matrices are links between the "vec" operator and "vech" operator: for an r by r symmetric matrix A,  $\operatorname{vech}(A) = \operatorname{Contr}(r)\operatorname{vec}(A)$ , and  $\operatorname{vec}(A) = \operatorname{Expan}(r)\operatorname{vech}(A)$ . The "vec" operator stacks the matrix A into an r^2 by 1 vector columnwise. The "vech" operator stacks the lower triangle or the upper triangle of a symmetric matrix into an r(r+1)/2 vector. For more details of "vec", "vech", contraction and expansion matrix, refer to Henderson and Searle (1979).

# 5 fit\_OLS

Multivariate linear regression.

#### Contents

- Usage
- Description

# Usage

[betaOLS SigmaOLS]=fit\_OLS(X,Y)

#### Input

- X: Predictors, an n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

#### Output

- beta OLS: An r by p matrix containing estimate of the regression coefficients  $\beta.$
- SigmaOLS: An r by r matrix containing estimate of the error covariance matrix.

## Description

In a multivariate linear model, Y and X follows the following relationship:  $Y = \alpha + \beta X + \varepsilon$ , where  $\varepsilon$  contains the errors. This function performs the ordinary least squares fit to the inputs, and returns the estimates of  $\beta$  and the covariance matrix of  $\varepsilon$ .

# 6 get\_Init

Starting value for the envelope subspace.

#### Contents

- Usage
- Description
- Reference

#### Usage

 $WInit=get\_Init(X,Y,u,dataParameter)$ 

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations.
- u: Dimension of the envelope. An integer between 1 and r-1.
- dataParameter: A list containing commonly used statistics computed from the data.

#### Output

• WInit: The initial estimate of the orthogonal basis of the envelope subspace. An r by u orthogonal matrix.

## Description

We compute the eigenvectors for the covariance matrices of Y and the estimated errors, and get 2r vectors. Then we get all the combinations of u vectors out of the 2r vectors. If the number of 2r choose u is small(<=50), we search over all the combinations and find out the one that minimizes the objective function F. If that number is large, then we do it iteratively: we pick up any u eigenvectors, fix all of them except the first one. Then we search over all the vectors orthogonal to the fixed ones, and record the one that minimizes F. Next, we fix the first u eigenvectors again but this time search for second one, then we record the vector. This goes on and on until the last one. We do it for 5 rounds and use the final set as our starting value.

#### Reference

The codes is implemented based on the algorithm in Section 3.5 of Su and Cook (2011).

# 7 Kpd

Compute the communication matrix Kpd.

## Contents

- Usage
- Description
- Reference

# Usage

k=Kpd(p,d)

Input

• p and d are two positive integers represent the dimension parameters for the communication matrix.

# Output

• k: The communication matrix Kpd. An p\*d by p\*d matrix.

# Description

For a p by d matrix A, vec(A') = Kpd\*vec(A), and Kpd is called a communication matrix.

### Reference

The codes is implemented based on Definition 3.1 in Magnus and Neudecker (1979).

# 8 Lmatrix

Extract the 2nd to the last diagonal element of a matrix into a vector.

## Contents

- Usage
- Description

# Usage

L=Lmatrix(r)

Input

• r: The dimension of the matrix being extracted. The matrix should be an r by r matrix.

Output

• L: An r-1 dimensional vector that contains all the diagonal elements but the first one of the matrix.

# Description

Let A be an r by r matrix, and vec be the vector operator, then  $\operatorname{Lmatrix}(r)^*\operatorname{vec}(A)$  will give the 2nd to the rth diagonal elements of A, arranged in a column vector.

# 9 make\_parameter

Compute summary statistics from the data.

#### Contents

- Usage
- Description

# Usage

 $dataParameter=make\_parameter(X,Y,method)$ 

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables, and r should be strictly greater than p.
- method: A string of characters indicating which member of the envelope family to be used, the choices can be 'env', 'ienv', 'henv' or 'senv'.

#### Output

data Parameter: A list that contains summary statistics computed from the data. The output list can vary from method to method.

- dataParameter.n: The number of observations in the data. A positive integer.
- dataParameter.ng: A p by 1 vector containing the number of observations in each group. p is the number of groups. Only for 'henv'.
- dataParameter.ncum: A p by 1 vector containing the total number of observations till this group. Only for 'henv'.
- dataParameter.ind: An n by 1 vector indicating the sequence of the observations after sorted by groups.
- dataParameter.p: The number of predictors or number of groups for 'henv'. A positive integer.
- dataParameter.r: The number of responses. A positive integer.
- dataParameter.XC: Centered predictors. An n by p matrix with the ith row being the ith observation of X subtracted by the mean of X. Only for 'env' and 'ienv'.
- dataParameter.YC: Centered responses. An n by r matrix with the ith row being the ith observation of Y subtracted by the mean of Y. Only for 'env' and 'ienv'.

- dataParameter.mX: The mean of predictors. A p by 1 vector. For all method except 'henv'.
- dataParameter.mY: The mean of responses. An r by 1 vector.
- dataParameter.mYg: An r by p matrix with the ith column being the sample mean of the ith group.
- dataParameter.sigX: The sample covariance matrix of X. A p by p matrix.
- dataParameter.sigY: The sample covariance matrix of Y. An r by r matrix.
- dataParameter.sigRes: For 'env', 'senv', 'ienv': The sample covariance matrix of the residuals from the ordinary least squares regression of Y on X. An r by r matrix. For 'henv', an r by r by p three dimensional matrix with the ith depth is the ith sample covariance matrix for the ith group.
- dataParameter.sigFit: The sample covariance matrix of the fitted value from the ordinary least squares regression of Y on X. An r by r matrix. Only for method 'ienv'.
- dataParameter.betaOLS: The regression coefficients from the ordinary least squares regression of Y on X. An r by p matrix. For all method except 'henv'.

# Description

This function computes statistics that will be used frequently in the estimation for each method.

# Part II

# env

# 10 aic\_env

Select the dimension of the envelope subspace using Akaike information criterion

#### Contents

- Usage
- Description
- Example

### Usage

```
u=aic\_env(X,Y)
```

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

### Output

• u: Dimension of the envelope. An integer between 0 and r.

## Description

This function implements the Akaike information criteria (AIC) to select the dimension of the envelope subspace.

```
load wheatprotein.txt
X=wheatprotein(:,8);
Y=wheatprotein(:,1:6);
u=aic_env(X,Y)
```

# 11 bic\_env

Select the dimension of the envelope subspace using Bayesian information criterion.

#### Contents

- Usage
- Description
- Example

# Usage

```
u=bic\_env(X,Y)
```

## Input

- X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

#### Output

• u: Dimension of the envelope. An integer between 0 and r.

# Description

This function implements the Bayesian information criteria (BIC) to select the dimension of the envelope subspace.

```
load wheatprotein.txt
X=wheatprotein(:,8);
Y=wheatprotein(:,1:6);
u=bic_env(X,Y)
```

# 12 bstrp\_env

Compute bootstrap standard error for the envelope model.

#### Contents

- Usage
- Description
- Example

## Usage

```
bootse=bstrp\_env(X,Y,B,u)
```

#### Input

- X: Predictors, an n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables
- B: Number of boostrap samples. A positive integer.
- u: Dimension of the envelope subspace. A positive integer between 0 and r.

## Output

• bootse: The standard error for elements in  $\beta$  computed by bootstrap. An r by p matrix.

## Description

This function computes the bootstrap standard errors for the regression coefficients in the envelope model by bootstrapping the residuals.

```
load wheatprotein.txt

X=wheatprotein(:,8);

Y=wheatprotein(:,1:6);

alpha=0.01;

u=lrt_env(Y,X,alpha)

B=100;

bootse=bstrp_env(X,Y,B,u)
```

# 13 dF4env

The first derivative of the objective funtion for computing the envelope subspace.

#### Contents

- Usage
- Description

# Usage

df = dF4env(R,dataParameter)

#### Input

- R: An r by u semi orthogonal matrix, 0<u<=r.
- dataParameter: A structure that contains the statistics calculated form the data.

#### Output

• df: An r by u containing the value of the derivative function evaluated at R.

# Description

The objective function is derived in Section 4.3 in Cook et al. (2010) by using maximum likelihood estimation. This function is the derivative of the objective function.

#### 14 env

Fit the envelope model.

#### Contents

- Usage
- Description
- References
- Example

#### Usage

stat = env(X,Y,u)

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables, and r should be strictly greater than p.
- u: Dimension of the envelope. An integer between 0 and r.

#### Output

stat: A list that contains the maximum likelihood estimators and some statistics.

- stat.beta: The envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- stat.Sigma: The envelope estimator of the error covariance matrix. An r by r matrix.
- stat.Gamma: The orthogonal basis of the envelope subspace. An r by u semi-orthogonal matrix.
- stat.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- stat.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix.
- stat.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.
- stat.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- stat.alpha: The estimated intercept in the envelope model. An r by 1 vector
- stat.l: The maximized log likelihood function. A real number.

- stat.asyEnv: Asymptotic standard error for elements in  $\beta$  under the envelope model. An r by p matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by  $1/\operatorname{sqrt}(n)$ .
- stat.ratio: The asymptotic standard error ratio of the standard multivariate linear regression estimator over the envelope estimator, for each element in  $\beta$ . An r by p matrix.
- stat.np: The number of parameters in the envelope model. A positive integer.

# Description

This function fits the envelope model to the responses and predictors, using the maximum likehood estimation. When the dimension of the envelope is between 1 and r-1, we implemented the algorithm in Cook et al. (2010). When the dimension is r, then the envelope model degenerates to the standard multivariate linear regression. When the dimension is 0, it means that X and Y are uncorrelated, and the fitting is different.

#### References

- The codes is implemented based on the algorithm in Section 4.3 of Cook et al (2010).
- The Grassmann manifold optimization step calls the package sg\_min 2.4.1 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

#### Example

The following codes will reconstruct the results in the wheat protein data example in Cook et al. (2010).

```
load wheatprotein.txt

X=wheatprotein(:,8);

Y=wheatprotein(:,1:6);

alpha=0.01;

u=lrt_env(Y,X,alpha)

stat=env(X,Y,u)

stat.Omega

eig(stat.Omega0)

stat.ratio
```

# 15 F4env

Objective funtion for computing the envelope subspace.

#### Contents

- Usage
- Description

# Usage

f = F4env(R,dataParameter)

Input

- R: An r by u semi orthogonal matrix, 0<u<=r.
- dataParameter: A structure that contains the statistics calculated form the data.

# Output

• f: A scalar containing the value of the objective function evaluated at R.

# Description

The objective function is derived in Section 4.3 of Cook et al. (2010) using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace.

# 16 lrt\_env

Select the dimension of the envelope subspace using likelihood ratio testing.

#### Contents

- Usage
- Description
- Example

# Usage

```
u=lrt_env(X,Y,alpha)
```

## Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.
- alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

#### Output

• u: Dimension of the envelope. An integer between 0 and r.

### Description

This function implements the likelihood ratio testing procedure to select the dimension of the envelope subspace, with prespecified significance level  $\alpha$ .

```
load wheatprotein.txt
X=wheatprotein(:,8);
Y=wheatprotein(:,1:6);
alpha=0.01;
u=lrt_env(Y,X,alpha)
```

# Part III

# henv

## 17 aic\_henv

Select the dimension of the envelope subspace using Akaike information criterion for the heteroscedastic envelope model.

#### Contents

- Usage
- Description
- Example

### Usage

 $u=aic\_henv(X,Y)$ 

Input

- X: Group indicators. An n by p matrix, p is the number of groups. X can only take p different values, one for each group.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

### Output

• u: Dimension of the envelope. An integer between 0 and r.

## Description

This function implements the Akaike information criteria (AIC) to select the dimension of the envelope subspace for the heteroscedastic envelope model.

## Example

load waterstrider.mat  $u=aic\_henv(X,Y)$ 

# 18 bic\_henv

Select the dimension of the envelope subspace using Bayesian information criterion for the heteroscedastic envelope model.

#### Contents

- Usage
- Description
- Example

# Usage

 $u=bic\_henv(X,Y)$ 

#### Input

- X: Group indicators. An n by p matrix, p is the number of groups. X can only take p different values, one for each group.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

#### Output

• u: Dimension of the envelope. An integer between 0 and r.

# Description

This function implements the Bayesian information criteria (BIC) to select the dimension of the envelope subspace for the heteroscedastic envelope model.

# Example

 $\begin{array}{l} load\ waterstrider.mat\\ u{=}bic\_henv(X,Y) \end{array}$ 

# 19 bstrp\_henv

Compute bootstrap standard error for the heteroscedastic envelope model.

#### Contents

- Usage
- Description
- Example

# Usage

 $bootse=bstrp\_henv(X,Y,B,u)$ 

### Input

- X: Group indicators. An n by p matrix, p is the number of groups. X can only take p different values, one for each group.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables
- B: Number of boostrap samples. A positive integer.
- u: Dimension of the envelope subspace. A positive integer between 0 and r.

#### Output

• bootse: The standard error for elements in  $\beta$  computed by bootstrap. An r by p matrix.

# Description

This function computes the bootstrap standard errors for the regression coefficients in the heteroscedastic envelope model by bootstrapping the residuals.

```
\label{eq:load_waterstrider.mat} \begin{split} & \text{load waterstrider.mat} \\ & u \!=\! \text{lrt\_henv}(X,\!Y,\!0.01) \\ & B \!=\! 100; \\ & \text{bootse=bstrp\_henv}(X,\!Y,\!B,\!u) \end{split}
```

# 20 dF4henv

The first derivative of the objective funtion for computing the envelope subspace in the heteroscedastic envelope model.

#### Contents

- Usage
- Description

# Usage

df = dF4henv(R,dataParameter)

## Input

- R: An r by u semi orthogonal matrix, 0<u<=r.
- dataParameter: A structure that contains the statistics calculated form the data.

#### Output

• df: An r by u containing the value of the derivative function evaluated at R.

# Description

The objective function is derived in Section 2.2 in Su and Cook (2012) by using maximum likelihood estimation. This function is the derivative of the objective function.

# 21 F4henv

Objective funtion for computing the envelope subspace in heteroscedastic envelope model.

#### Contents

- Usage
- Description

# Usage

f = F4henv(R,dataParameter)

#### Input

- R: An r by u semi orthogonal matrix, 0<u<=r.
- dataParameter: A structure that contains the statistics calculated form the data.

#### Output

• f: A scalar containing the value of the objective function evaluated at R.

# Description

The objective function is derived in Section 2.2 of Su and Cook (2012) using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace in the heteroscedastic envelope model.

# 22 henv

Fit the heteroscedastic envelope model.

#### Contents

- Usage
- Description
- References
- Example

#### Usage

stat=henv(X,Y,u)

#### Input

- X: Group indicators. An n by p matrix, p is the number of groups. X can only take p different values, one for each group.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables, and r should be strictly greater than p.
- u: Dimension of the envelope. An integer between 0 and r.

#### Output

stat: A list that contains the maximum likelihood estimators and some statistics.

- stat.mu: The heteroscedastic envelope estimator of the grand mean. A r by 1 vector.
- stat.mug: The heteroscedastic envelope estimator of the group mean. A r by p matrix, the ith column of the matrix contains the mean for the ith group.
- stat.Yfit: A n by r matrix, the ith row gives the group mean of the group that the ith observation belongs to. As X is just a group indicator, and is not ordinal, stat.mug alone does not tell which group corresponds to which group mean.
- stat.Gamma: The orthogonal basis of the envelope subspace. An r by u semi-orthogonal matrix.
- stat.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- stat.beta: The heteroscedastic envelope estimator of the group mean effect. An r by p matrix, the ith column of the matrix contains the main effect for the ith group.

- stat.Sigma: The heteroscedastic envelope estimator of the error covariance matrix. A three dimensional matrix with dimension r, r and p, stat.Sigma(:,:,i) contains the estimated covariance matrix for the ith group.
- stat.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix, the ith column contains the coordinates of the main effect of the ith group with respect to Gamma.
- stat.Omega: The coordinates of Sigma with respect to Gamma. An u by u by p matrix, stat.Omega(:,:,i) contains the coordinates of the covariance matrix of the ith group with respect to Gamma.
- stat.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- stat.l: The maximized log likelihood function. A real number.
- stat.np: The number of parameters in the heteroscedastic envelope model. A positive integer.
- stat.asyHenv: The asymptotic standard errors for elements in *beta* under the heteroscedastic envelope model. An r by p matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by 1/sqrt(n).
- stat.ratio: The asymptotic standard error ratio of the standard multivariate linear regression estimator over the heteroscedastic envelope estimator. An r by p matrix, the (i, j)th element in stat.ratio is the elementwise standard error ratio for the ith element in the jth group mean effect.

# Description

This function fits the heteroscedatic envelope model to the responses and predictors, using the maximum likehood estimation. When the dimension of the envelope is between 1 and r-1, we implemented the algorithm in Su and Cook (2012). When the dimension is r, then the envelope model degenerates to the standard multivariate linear model for comparing group means. When the dimension is 0, it means there is not any group effect, and the fitting is different.

#### References

- The codes is implemented based on the algorithm in Section 2.2 of Su and Cook (2012).
- The Grassmann manifold optimization step calls the package sg\_min 2.4.1 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

#### Example

The following codes produce the results of the waterstrider example in Su and Cook (2011).

 $\begin{array}{l} load\ waterstrider.mat\\ u=lrt\_henv(X,Y,0.01)\\ stat=henv(X,Y,u)\\ stat.ratio \end{array}$ 

# 23 lrt\_henv

Select the dimension of the envelope subspace using likelihood ratio testing for the heteroscedastic envelope model.

#### Contents

- Usage
- Description
- Example

### Usage

 $u=lrt\_henv(X,Y,alpha)$ 

#### Input

- X: Group indicators. An n by p matrix, p is the number of groups. X can only take p different values, one for each group.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.
- alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

#### Output

• u: Dimension of the envelope. An integer between 0 and r.

## Description

This function implements the likelihood ratio testing procedure to select the dimension of the envelope subspace in heteroscedastic envelope model, with prespecified significance level  $\alpha$ .

# Example

load waterstrider.mat  $u=lrt\_henv(X,Y,0.01)$ 

# Part IV

# ienv

# 24 aic\_ienv

Select the dimension of the inner envelope subspace using Akaike information criterion.

#### Contents

- Usage
- Description
- Example

# Usage

 $u=aic\_ienv(X,Y)$ 

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

#### Output

• u: Dimension of the inner envelope. An integer between 0 and p or equal to r.

# Description

This function implements the Akaike information criteria (AIC) to select the dimension of the inner envelope subspace.

# Example

 $\begin{array}{l} load\ irisf.mat\\ u{=}aic\_ienv(X,Y) \end{array}$ 

# 25 bic\_ienv

Select the dimension of the inner envelope subspace using Bayesian information criterion.

#### Contents

- Usage
- Description
- Example

# Usage

 $u=bic\_ienv(X,Y)$ 

## Input

- X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

## Output

• u: Dimension of the inner envelope. An integer between 0 and p or equal to r.

## Description

This function implements the Bayesian information criteria (BIC) to select the dimension of the inner envelope subspace.

# Example

load irisf.mat $u=bic\_ienv(X,Y)$ 

# 26 bstrp\_ienv

Compute bootstrap standard error for the inner envelope model.

#### Contents

- Usage
- Description
- Example

# Usage

 $bootse=bstrp\_ienv(X,Y,B,u)$ 

#### Input

- X: Predictors, an n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables
- B: Number of boostrap samples. A positive integer.
- u: Dimension of the inner envelope. An integer between 0 and p or equal to r.

#### Output

• bootse: The standard error for elements in  $\beta$  computed by bootstrap. An r by p matrix.

# Description

This function computes the bootstrap standard errors for the regression coefficients in the inner envelope model by bootstrapping the residuals.

```
load irisf.mat
```

```
\label{eq:control_equation} \begin{split} u&=\text{bic\_ienv}(X,Y)\\ B&=100;\\ bootse&=bstrp\_ienv(X,Y,B,u) \end{split}
```

# 27 dF4ienv

First derivative of the objective funtion for computing the inner envelope subspace.

#### Contents

- Usage
- Description

# Usage

f = dF4ienv(R,dataParameter)

#### Input

- R: An r by u semi-orthogonal matrix, 0<u<=p.
- dataParameter: A structure that contains the statistics calculated form the data.

#### Output

• dF: The first derivative of the objective function for computing the inner envelope subspace. An r by u matrix.

# Description

This first derivative of F4ienv obtained by matrix calculus calculations.

# 28 F4ienv

Objective funtion for computing the inner envelope subspace

#### Contents

- Usage
- Description

# Usage

f = F4ienv(R,dataParameter)

Input

- R: An r by u semi orthogonal matrix, 0<u<=p.
- dataParameter: A structure that contains the statistics calculated form the data.

# Output

• f: A scalar containing the value of the objective function evaluated at R.

# Description

The objective function is derived in Section 3.3 in Su and Cook (2012) by using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated inner envelope subspace.

### 29 ienv

Fit the inner envelope model.

#### Contents

- Usage
- Description
- References
- Example

## Usage

stat = ienv(X,Y,u)

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables, and r should be strictly greater than p.
- u: Dimension of the inner envelope. An integer between 0 and p or equal to r.

#### Output

stat: A list that contains the maximum likelihood estimators and some statistics.

- stat.beta: The envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- stat.Sigma: The envelope estimator of the error covariance matrix. An r by r matrix.
- stat.Gamma1: The orthogonal basis of the inner envelope subspace. An r by u semi-orthogonal matrix.
- stat.Gamma0: The orthogonal basis of the complement of the inner envelope subspace. An r by r-u semi-orthogonal matrix.
- stat.eta1: The transpose of the coordinates of  $\beta$  with respect to Gamma1. An p by u matrix.
- $\bullet$  stat.B: An (r-u) by (p-u) semi-orthogonal matrix, so that (Gamma, Gamma0\*B) spans  $\beta.$
- stat.eta2: The transpose of the coordinates of  $\beta$  with respect to Gamma0. An p by (p-u) matrix.
- stat.Omega1: The coordinates of Sigma with respect to Gamma1. An u by u matrix.

- stat.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- stat.alpha: The estimated intercept in the inner envelope model. An r by 1 vector.
- stat.l: The maximized log likelihood function. A real number.
- stat.asylenv: Asymptotic standard error for elements in  $\beta$  under the inner envelope model. An r by p matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by  $1/\operatorname{sqrt}(n)$ .
- stat.ratio: The asymptotic standard error ratio of the stanard multivariate linear regression estimator over the inner envelope estimator, for each element in  $\beta$ . An r by p matrix.
- stat.np: The number of parameters in the inner envelope model. A positive integer.

# Description

This function fits the inner envelope model to the responses and predictors, using the maximum likehood estimation. When the dimension of the envelope is between 1 and p-1, we implemented the algorithm in Su and Cook (2012). When the dimension is p, then the inner envelope model degenerates to the standard multivariate linear regression. When the dimension is 0, it means that X and Y are uncorrelated, and the fitting is different.

### References

- The codes is implemented based on the algorithm in Su and Cook (2012).
- The Grassmann manifold optimization step calls the package sg\_min 2.4.1 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

### Example

The following codes gives the results of the Fisher's iris data example in Su and Cook (2012).

load irisf.mat

 $\begin{array}{l} u=& bic\_env(X,Y) \\ d=& bic\_ienv(X,Y) \\ stat=& ienv(X,Y,d) \\ 1-1./stat.ratio \end{array}$ 

# 30 lrt\_ienv

Select the dimension of the inner envelope subspace using likelihood ratio testing.

#### Contents

- Usage
- Description
- Example

## Usage

 $u=lrt\_ienv(X,Y,alpha)$ 

### Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.
- alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

### Output

 $\bullet$ u: Dimension of the inner envelope. An integer between 0 and p or equal to r.

# Description

This function implements the likelihood ratio testing procedure to select the dimension of the inner envelope subspace, with prespecified significance level  $\alpha$ .

```
load irisf.mat
```

```
\begin{array}{l} alpha{=}0.01;\\ u{=}lrt\_ienv(X,Y,alpha) \end{array}
```

# Part V

# penv

# 31 aic\_penv

Select the dimension of the partial envelope subspace using Akaike information criterion.

### Contents

- Usage
- Description
- Example

## Usage

```
u=aic\_penv(X1,X2,Y)
```

#### Input

- X1: Predictors of main interst. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X2: Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

### Output

• u: Dimension of the envelope. An integer between 0 and r.

# Description

This function implements the Akaike information criteria (AIC) to select the dimension of the partial envelope subspace.

```
load T7-7.dat
Y=T7_7(:,1:4);
X=T7_7(:,5:7);
```

```
\begin{array}{l} X1{=}X(:,\!3); \\ X2{=}X(:,\!1{:}2); \\ u{=}aic\_penv(X1,\!X2,\!Y) \end{array}
```

# 32 bic\_penv

Select the dimension of the partial envelope subspace using Bayesian information criterion.

#### Contents

- Usage
- Description
- Example

## Usage

```
u=bic_penv(X1,X2,Y)
```

### Input

- X1: Predictors of main interst. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X2: Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

### Output

• u: Dimension of the envelope. An integer between 0 and r.

# Description

This function implements the Bayesian information criteria (BIC) to select the dimension of the partial envelope subspace.

```
\begin{array}{l} {\rm load\ T7\text{-}7.dat} \\ Y{=}T7\text{-}7(:,1:4); \\ X{=}T7\text{-}7(:,5:7); \\ X1{=}X(:,3); \\ X2{=}X(:,1:2); \\ u{=}{\rm bic\_penv}(X1,X2,Y) \end{array}
```

# 33 bstrp\_penv

Compute bootstrap standard error for the partial envelope model.

#### Contents

- Usage
- Description
- Example

# Usage

```
bootse=bstrp_penv(X1,X2,Y,B,u)
```

# Input

- X1: Predictors of main interst. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X2: Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates. The covariates can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.
- B: Number of boostrap samples. A positive integer.
- u: Dimension of the partial envelope subspace. A positive integer between 0 and r.

## Output

• bootse: The standard error for elements in  $\beta_1$  computed by bootstrap. An r by p1 matrix.

# Description

This function computes the bootstrap standard errors for the regression coefficients in the partial envelope model by bootstrapping the residuals.

```
load T7-7.dat
Y=T7<sub>-</sub>7(:,1:4);
X=T7<sub>-</sub>7(:,5:7);
```

```
\begin{array}{l} {\rm X1{=}X(:,3);} \\ {\rm X2{=}X(:,1{:}2);} \\ {\rm alpha{=}0.01;} \\ {\rm u{=}lrt\_penv}({\rm X1{,}X2{,}Y{,}alpha}) \\ {\rm B}{=}100; \\ {\rm bootse{=}bstrp\_penv}({\rm X1{,}X2{,}Y{,}B{,}u}) \end{array}
```

# $34 \quad lrt_{-penv}$

Select the dimension of the partial envelope subspace using likelihood ratio testing.

#### Contents

- Usage
- Description
- Example

## Usage

```
u=lrt\_penv(X1,X2,Y,alpha)
```

### Input

- X1: Predictors of main interst. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X2: Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates.
- Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.
- $\bullet$  alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

#### Output

 $\bullet$ u: Dimension of the partial envelope subspace. An integer between 0 and r.

# Description

This function implements the likelihood ratio testing procedure to select the dimension of the partial envelope subspace, with prespecified significance level  $\alpha$ .

```
load T7-7.dat
Y=T7_7(:,1:4);
X=T7_7(:,5:7);
X1=X(:,3);
```

```
\begin{array}{l} {\rm X2{=}X(:,1:2);} \\ {\rm alpha{=}0.01;} \\ {\rm u{=}lrt{\_}penv}({\rm X1,X2,Y,alpha}) \end{array}
```

# 35 penv

Fit the partial envelope model.

#### Contents

- Usage
- Description
- References
- Example

## Usage

stat=penv(X1,X2,Y,u)

#### Input

- X1: Predictors of main interst. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X2: Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates. The covariates can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables, and r should be strictly greater than p1.
- u: Dimension of the partial envelope. An integer between 0 and r.

### Output

stat: A list that contains the maximum likelihood estimators and some statistics.

- stat.beta1: The partial envelope estimator of  $\beta_1$ , which is the regression coefficients for X1. An r by p1 matrix.
- stat.beta2: The partial envelope estimator of  $\beta_2$ , which is the regression coefficients for X2. An r by p2 matrix.
- stat.Sigma: The partial envelope estimator of the error covariance matrix. An r by r matrix.
- stat.Gamma: The orthogonal basis of the partial envelope subspace. An r by u semi-orthogonal matrix.
- stat.Gamma0: The orthogonal basis of the complement of the partial envelope subspace. An r by r-u semi-orthogonal matrix.
- stat.eta: The coordinates of  $\beta_1$  with respect to Gamma. An u by p1 matrix.

- stat.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.
- stat.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- stat.alpha: The estimated intercept in the partial envelope model. An r by 1 vector.
- stat.l: The maximized log likelihood function. A real number.
- stat.asyPenv: Asymptotic standard error for elements in  $\beta$  under the partial envelope model. An r by p1 matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by  $1/\operatorname{sqrt}(n)$ .
- stat.ratio: The asymptotic standard error ratio of the stanard multivariate linear regression estimator over the partial envelope estimator, for each element in  $\beta_1$ . An r by p1 matrix.
- stat.np: The number of parameters in the envelope model. A positive integer.

# Description

This function fits the partial envelope model to the responses Y and predictors X1 and X2, using the maximum likehood estimation. When the dimension of the envelope is between 1 and r-1, we implemented the algorithm in Su and Cook (2011). When the dimension is r, then the partial envelope model degenerates to the standard multivariate linear regression with Y as the responses and both X1 and X2 as predictors. When the dimension is 0, X1 and Y are uncorrelated, and the fitting is the standard multivariate linear regression with Y as the responses and X2 as the predictors.

### References

- The codes is implemented based on the algorithm in Section 3.2 of Su and Cook (2012).
- The Grassmann manifold optimization step calls the package sg\_min 2.4.1 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

### Example

The following codes reconstruct the results of the paper and fiber example in Su and Cook (2012).

```
\begin{array}{l} {\rm load\ T7\text{-}7.dat} \\ {\rm Y=T7\text{-}7(:,1:4);} \\ {\rm X=T7\text{-}7(:,5:7);} \\ {\rm X1=X(:,3);} \\ {\rm X2=X(:,1:2);} \\ {\rm alpha=0.01;} \\ {\rm u=lrt\_penv(X1,X2,Y,alpha)} \end{array}
```

 $\begin{array}{l} stat{=}penv(X1{,}X2{,}Y{,}u)\\ stat{.}Omega\\ eig(stat{.}Omega0)\\ stat{.}ratio \end{array}$ 

# Part VI

# senv

# 36 aic\_senv

Select the dimension of the scaled envelope subspace using Akaike information criterion.

### Contents

- Usage
- Description
- Example

## Usage

```
u=aic\_senv(X,Y)
```

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

## Output

• u: Dimension of the inner envelope. An integer between 0 and r.

# Description

This function implements the Akaike information criteria (AIC) to select the dimension of the scaled envelope subspace.

```
load('T9-12.txt')
Y=T9_12(:,4:7);
X=T9_12(:,1:3);
u=aic_senv(X,Y)
```

# 37 bic\_senv

Select the dimension of the scaled envelope subspace using Bayesian information criterion.

### Contents

- Usage
- Description
- Example

# Usage

```
u=bic\_senv(X,Y)
```

# Input

- X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

## Output

• u: Dimension of the inner envelope. An integer between 0 and r.

# Description

This function implements the Bayesian information criteria (BIC) to select the dimension of the scaled envelope subspace.

```
\begin{array}{l} load('T9\text{-}12.txt') \\ Y {=} T9\text{-}12(:,4\text{:}7); \\ X {=} T9\text{-}12(:,1\text{:}3); \\ u {=} bic\_senv(X,Y) \end{array}
```

# 38 bstrp\_senv

Compute bootstrap standard error for the scaled envelope model.

#### Contents

- Usage
- Description
- Example

## Usage

```
bootse=bstrp\_senv(X,Y,B,u)
```

# Input

- X: Predictors, an n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables
- B: Number of boostrap samples. A positive integer.
- u: Dimension of the envelope subspace. A positive integer between 0 and r.

### Output

• bootse: The standard error for elements in  $\beta$  computed by bootstrap. An r by p matrix.

# Description

This function computes the bootstrap standard errors for the regression coefficients in the scaled envelope model by bootstrapping the residuals.

```
\begin{split} & \text{load}(\text{'T9-12.txt'}) \\ & Y = \text{T9\_12}(:,4:7); \\ & X = \text{T9\_12}(:,1:3); \\ & u = \text{bic\_ienv}(X,Y) \\ & B = 20; \\ & \text{bootse} = \text{bstrp\_senv}(X,Y,B,u) \end{split}
```

# 39 dF4senv

First derivative of the objective funtion for computing the envelope subspace in the scaled envelope model.

### Contents

- Usage
- Description

# Usage

f = dF4senv(R,dataParameter)

### Input

- R: An r by u semi-orthogonal matrix, 0<u<=p.
- dataParameter: A structure that contains the statistics calculated form the data.

### Output

• dF: The first derivative of the objective function for computing the envelope subspace. An r by u matrix.

# Description

This first derivative of F4senv obtained by matrix calculus calculations.

# 40 F4senv

Objective funtion for computing the envelope subspace in scaled envelope model.

### Contents

- Usage
- Description

# Usage

f = F4senv(R,dataParameter)

### Input

- R: An r by u semi orthogonal matrix, 0<u<r.
- data Parameter: A structure that contains the statistics calculated form the data.

### Output

• f: A scalar containing the value of the objective function evaluated at R.

# Description

The objective function is derived in Section 4.1 in Cook and Su (2012) using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace.

# 41 objfun

Objective funtion for computing the scales in the scaled envelope model.

### Contents

- Usage
- Description

# Usage

f = objfun(d,Gamma,dataParameter)

#### Input

- d: An r-1 dimensional column vector containing the scales for the 2nd to the rth responses. All the entries in d are positive.
- Gamma: A r by u semi-orthogomal matrix that spans the envelope subspace or the estimated envelope subspace.
- dataParameter: A structure that contains the statistics calculated form the data.

### Output

• f: A scalar containing the value of the objective function evaluated at d.

# Description

The objective function is derived in Section 4.1 of Su and Cook (2012) using maximum likelihood estimation.

# 42 senv

Fit the scaled envelope model.

#### Contents

- Usage
- Description
- References
- Example

## Usage

stat=senv(X,Y,u)

#### Input

- X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.
- Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables, and r should be strictly greater than p.
- u: Dimension of the envelope. An integer between 0 and r.

#### Output

stat: A list that contains the maximum likelihood estimators and some statistics.

- stat.beta: The scaled envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- stat.Sigma: The scaled envelope estimator of the error covariance matrix. An r by r matrix.
- stat.Lambda: The matrix of estimated scales. An r by r diagonal matrix with the first diagonal element equal to 1 and other diagonal elements being positive.
- stat.Gamma: The orthogonal basis of the envelope subspace. An r by u semi-orthogonal matrix.
- stat.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- stat.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix.
- stat.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.
- stat.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.

- stat.alpha: The estimated intercept in the scaled envelope model. An r by 1 vector.
- stat.l: The maximized log likelihood function. A real number.
- stat.asySenv: Asymptotic standard error for elements in  $\beta$  under the scaled envelope model. An r by p matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by  $1/\operatorname{sqrt}(n)$ .
- stat.ratio: The asymptotic standard error ratio of the standard multivariate linear regression estimator over the scaled envelope estimator, for each element in  $\beta$ . An r by p matrix.
- stat.np: The number of parameters in the scaled envelope model. A positive integer.

# Description

This function fits the scaled envelope model to the responses and predictors, using the maximum likehood estimation. When the dimension of the envelope is between 1 and r-1, we implemented the algorithm in Cook and Su (2012). When the dimension is r, then the scaled envelope model degenerates to the standard multivariate linear regression. When the dimension is 0, it means that X and Y are uncorrelated, and the fitting is different.

#### References

- The codes is implemented based on the algorithm in Section 4.1 of Cook and Su (2012).
- The Grassmann manifold optimization step calls the package sg\_min 2.4.1 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

## Example

The following codes produce the results of the test and performance example in Cook and Su (2012).

```
load('T9-12.txt')
Y=T9.12(:,4:7);
X=T9.12(:,1:3);
u=bic_env(X,Y)
stat=env(X,Y,u);
1-1./stat.ratio
u=bic_senv(X,Y)
stat=senv(X,Y,u);
statLambda
1-1./stat.ratio
```