# MATLAB Toolbox Envelope: Reference Manual

## June 3, 2012

Co	Contents 1							
1	tools	8	2					
	1.1	bootstrapse	2					
	1.2	bootstrapse_OLS	5					
	1.3	mfoldcv	7					
	1.4	modelselectaic	9					
	1.5	modelselectbic	11					
	1.6	modelselectlrt	13					
	1.7	prediction	15					
	1.8	testcoefficient	18					
2	env		20					
	2.1	aic_env	20					
	2.2	bic_env	22					
	2.3	bstrp_env	24					
	2.4	dF4env	26					
	2.5	env	27					
	2.6	F4env	31					
	2.7	lrt_env	32					
	2.8	predict_env	34					
	2.9	testcoefficient_env	37					
	2.3	testcoemcient_env	31					
3	envpls 39							
	3.1	bstrp_envpls	39					
	3.2	envpls	41					
	3.3	mfoldcv_xenvpls	44					
4	henv 46							
	4.1	aic_henv	46					
	4.2	bic_henv	48					
	4.3	bstrp_henv	50					
	4.4	dF4henv	52					
	4.5	F4henv	53					
	4.6	henv	54					
	4.7	lrt_henv	57					
	4.8	predict_henv	59					
	4.9	testcoefficient_henv	62					

2 CONTENTS

5	ienv		<b>64</b>
	5.1	aic_ienv	64
	5.2	bic_ienv	66
	5.3	bstrp_ienv	67
	5.4	dF4ienv	69
	5.5	F4ienv	70
	5.6	ienv	71
	5.7		74
		lrt_ienv	
	5.8	predict_ienv	76
	5.9	testcoefficient_ienv	78
6	penv		80
	6.1	aic_penv	80
	6.2	bic_penv	82
	6.3	bstrp_penv	84
	6.4	lrt_penv	86
	6.5	penv	88
	6.6	predict_penv	91
	6.7	testcoefficient_penv	94
	0.7	testcoemcient_penv	94
7	senv		96
	7.1	aic_senv	96
	7.2	bic_senv	98
	7.3	bstrp_senv	100
	7.4	dF4senv	102
	7.5		103
	7.6		104
	7.7		105
	7.8	· –	107
	7.0 7.9		1107
	7.9	testcoefficient_senv	110
8	xenv		112
	8.1	aic_xenv	112
	8.2	bic_xenv	114
	8.3	bstrp_xenv	116
	8.4	•	118
	8.5		119
	8.6		120
	8.7	<del>-</del>	122
		F	124
	8.8	<del>-</del>	
	8.9	xenv	126
9	xenv	pls	130
	9.1	bstrp_xenvpls	130
	9.2	mfoldcv_xenvpls	132
	9.3	•	134
		•	
10	auxil	•	137
	10.1	center	137
	10.2	Contr	138
	10.3	Expan	139
		1	140

CONTENTS 3

10.5 get_envelope	142
10.6 get_Init	143
10.7 get_Init4henv	144
10.8 Kpd	145
10.9 Lmatrix	146
10.10 make_dF	147
10.11 make_F	148
10.12 make_opts	149
10.13 make_parameter	150
10.14 mtest	152

## tools

## 1.1 bootstrapse

Perform bootstrap to estimate actual standard errors for models in the envelope family.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
bootse = bootstrapse(X, Y, u, B, modelType)
bootse = bootstrapse(X, Y, u, B, modelType, Opts)
```

#### Input

X: Predictors. The predictors can be univariate or multivariate, discrete or continuous.

For model type for method 'env', 'envpls', 'henv', 'ienv', 'senv', 'xenv' and 'xenvpls'. X is an n by p matrix, p is the number of predictors.

For model type 'penv', X is A list containing the value of X1 and X2.

- X.X1 (only for 'penv'): Predictors of main interest. 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.
- X.X2 (only for 'penv'): 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.
- ${\bf u}$ : Dimension of the envelope subspace. The legitimate range of u depends on the model specified.
- **B**: Number of bootstrap samples. A positive integer.

**modelType**: A string characters indicting the model, choices can be 'env', 'envpls', 'henv', 'ienv', 'penv', 'senv', 'xenv' and 'xenvpls'.

1.1. BOOTSTRAPSE 5

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### Output

bootse: For 'env', 'envpls', 'henv', 'ienv', and 'senv', an r by p matrix containing the standard errors for elements in  $\beta$  computed by bootstrap. For 'penv', an r by p1 matrix containing the standard errors for  $\beta_1$  computed by bootstrap. For 'xenv' and 'xenvpls', a p by r matrix containing the standard errors for elements in  $\beta$  computed by bootstrap.

#### **Description**

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

```
load wheatprotein.txt
       X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1:6);
       alpha = 0.01;
       u = lrt_{env}(X, Y, alpha);
       B = 100;
       modelType = 'env';
       bootse = bootstrapse(X, Y, u, B, modelType)
bootse =
    0.2896
    0.4352
    0.3189
    0.5735
    0.2543
    0.5840
       modelType = 'envpls';
       bootse = bootstrapse(X, Y, u, B, modelType)
bootse =
    9.3899
```

```
7.7384
8.3303
9.0875
13.4416
5.1477

load fiberpaper.dat
    Y = fiberpaper(:, 1 : 4);
    Xtemp = fiberpaper(:, 5 : 7);
    X.X1 = Xtemp(:, 3);
    X.X2 = Xtemp(:, 1 : 2);
    alpha = 0.01;
    u = lrt_penv(X, Y, alpha);
    B = 100;
    modelType = 'penv';
    bootse = bootstrapse(X, Y, u, B, modelType)
```

bootse =

0.0027

0.0012

0.0020

0.0009

## 1.2 bootstrapse\_OLS

Compute bootstrap standard error for ordinary least squares.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
bootse = bootstrapse_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 bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter. If not defined, the default setting is used.

• Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### 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 ordinary least squares by bootstrapping the residuals.

```
load wheatprotein.txt
   X = wheatprotein(:, 8);
   Y = wheatprotein(:, 1 : 6);
   bootse = bootstrapse_OLS(X, Y, 200)

bootse =

10.2168
```

8.3940

9.0503

9.9677

14.5822

5.5874

1.3. MFOLDCV 9

## 1.3 mfoldcy

Select the dimension for the envelope family using m-fold cross validation.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = mfoldcv(X, Y, m, modelType)
u = mfoldcv(X, Y, m, modelType, Opts)
```

## Input

X: 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.

m: A positive integer that is used to indicate m-fold cross validation.

modelType: A string characters indicting the model, choices can be 'envpls' or 'xenvpls'.

**Opts**: A list containing the optional input parameters. If one or several (even all) fields are not defined, the default settings are used.

• Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### Output

**u**: The dimension of the envelope subspace selected by m-fold cross validation.

#### **Description**

This function implements m-fold cross validation to select the dimension of the envelope space, based on prediction performance. For each u, the data is partitioned into m parts, each part is in turn used for testing for the prediction performance while the rest m-1 parts are used for training. The dimension is select as the one that minimizes the average prediction errors. If Y is multivariate, the identity inner product is used for computing the prediction errors.

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1 : 6);
m = 5;
```

```
modelType = 'envpls';
u = mfoldcv(X, Y, m, modelType)
```

u =

0

## 1.4 modelselectaic

Select the dimension for the envelope family using Akaike information criteria.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = modelselectaic(X, Y, modelType)
u = modelselectaic(X, Y, modelType, Opts)
```

#### Input

X: Predictors. The predictors can be univariate or multivariate, discrete or continuous.

For model type for method 'env', 'henv', 'ienv', 'senv', and 'xenv'. X is an n by p matrix, p is the number of predictors.

For model type 'penv', X is A list containing the value of X1 and X2.

- X.X1 (only for 'penv'): Predictors of main interest. 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.
- X.X2 (only for 'penv'): 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.

**modelType**: A string characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv', 'senv' and 'xenv'.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

## 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 method 'env', 'henv', 'ienv', 'penv', ' senv', and 'xenv'.

```
load wheatprotein.txt
       X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1 : 6);
       modelType = 'env';
       u = modelselectaic(X, Y, modelType)
u =
    1
       load fiberpaper.dat
       Y = fiberpaper(:, 1 : 4);
       Xtemp = fiberpaper(:, 5 : 7);
       X.X1 = Xtemp(:, 3);
       X.X2 = Xtemp(:, 1 : 2);
       modelType = 'penv';
       u = modelselectaic(X, Y, modelType)
u =
     3
```

## 1.5 modelselectbic

Select the dimension for the envelope family using Bayesian information criteria.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = modelselectbic(X, Y, modelType)
u = modelselectbic(X, Y, modelType, Opts)
```

#### Input

X: Predictors. The predictors can be univariate or multivariate, discrete or continuous.

For model type for method 'env', 'henv', 'ienv', 'senv', and 'xenv'. X is an n by p matrix, p is the number of predictors.

For model type 'penv', X is A list containing the value of X1 and X2.

- X.X1 (only for 'penv'): Predictors of main interest. 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.
- X.X2 (only for 'penv'): 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.

**modelType**: A string characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv', 'senv' and 'xenv'.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

## 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 method 'env', 'henv', 'ienv', 'penv', ' senv', and 'xenv'.

```
load wheatprotein.txt
       X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1 : 6);
       modelType = 'env';
       u = modelselectbic(X, Y, modelType)
u =
    1
       load fiberpaper.dat
       Y = fiberpaper(:, 1 : 4);
       Xtemp = fiberpaper(:, 5 : 7);
       X.X1 = Xtemp(:, 3);
       X.X2 = Xtemp(:, 1 : 2);
       modelType = 'penv';
       u = modelselectbic(X, Y, modelType)
u =
     1
```

## 1.6 modelselectlrt

Select the dimension for the envelope family using likelihood ratio testing procedure.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = modelselectlrt(X, Y, alpha, modelType)
u = modelselectlrt(X, Y, alpha, modelType, Opts)
```

#### Input

X: Predictors. The predictors can be univariate or multivariate, discrete or continuous.

For model type for method 'env', 'henv', 'ienv', and 'xenv'. X is an n by p matrix, p is the number of predictors.

For model type 'penv', X is A list containing the value of X1 and X2.

- X.X1 (only for 'penv'): Predictors of main interest. 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.
- X.X2 (only for 'penv'): 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.

alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

**modelType**: A string characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv' and 'xenv'.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value:

#### 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 for method 'env', 'henv', 'ienv', 'penv', and 'xenv'. The likelihood ratio resting procedure does not support 'senv', because the scaled envelope models are not nested with the standard model.

```
load wheatprotein.txt
       X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1 : 6);
       alpha = 0.01;
       modelType = 'env';
       u = modelselectlrt(X, Y, alpha, modelType)
u =
     1
       load fiberpaper.dat
       Y = fiberpaper(:, 1 : 4);
       Xtemp = fiberpaper(:, 5 : 7);
       X.X1 = Xtemp(:, 3);
       X.X2 = Xtemp(:, 1 : 2);
       alpha = 0.01;
       modelType = 'penv';
       u = modelselectlrt(X, Y, alpha, modelType)
u =
     1
```

1.7. PREDICTION 17

## 1.7 prediction

Perform estimation or prediction for models in the envelope family.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

PredictOutput = prediction(ModelOutput, Xnew, infType, modelType)

#### **Input**

**ModelOutput**: A list containing the model outputs from fitting the models.

**Xnew**: The value of X with which to estimate or predict Y.

For 'env', 'henv', 'ienv', 'senv' and 'xenv', it is a p by 1 vector.

For 'penv', it is a list containing the value of X1 and X2.

\* Xnew.X1 (only for 'penv'): A p1 by 1 vector containing the value of X1. \* Xnew.X2 (only for 'penv'): A p2 by 1 vector containing the value of X2.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

**modelType**: A string characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv', 'senv' and 'xenv'.

## Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix.
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

## **Description**

This function evaluates the user-specified model, could be 'env', 'henv', 'ienv', 'penv', 'senv' or 'xenv', at new value Xnew. It can perform estimation: find the fitted value when X = Xnew, or prediction: predict Y when X = Xnew. The covariance matrix and the standard errors are also provided.

```
load wheatprotein.txt
      X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1:6);
       modelType = 'env';
       u = modelselectbic(X, Y, modelType);
       ModelOutput = env(X, Y, u);
       Xnew = X(2, :)';
       PredictOutput = predict_env(ModelOutput, Xnew, 'estimation')
       [PredictOutput.value, Y(2, :)'] % Compare the fitted value with
       the observed value
PredictOutput =
        value: [6x1 double]
    covMatrix: [6x6 double]
          SE: [6x1 double]
ans =
  474.7135 458.0000
  127.4740 112.0000
  251.2044 236.0000
  380.8280 368.0000
  380.9473 383.0000
  -6.3287 -15.0000
       load fiberpaper.dat
       Y = fiberpaper(:, 1 : 4);
      Xtemp = fiberpaper(:, 5 : 7);
      X.X1 = Xtemp(:, 3);
      X.X2 = Xtemp(:, 1 : 2);
       modelType = 'penv';
       u = modelselectbic(X, Y, modelType);
       ModelOutput = penv(X, Y, u);
       Xnew.X1 = X.X1(1, :)';
       Xnew.X2 = X.X2(1, :)';
       PredictOutput = predict_penv(ModelOutput, Xnew, 'estimation')
       PredictOutput.SE
PredictOutput =
       value: [4x1 double]
    covMatrix: [4x4 double]
```

1.7. PREDICTION 19

SE: [4x1 double]

ans =

1.4680

0.4234

0.7145

0.3161

## 1.8 testcoefficient

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\sim$ = A, where beta is estimated under the model in the envelope family.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
TestOutput = testcoefficient(ModelOutput, modelType)
TestOutput = testcoefficient(ModelOutput, modelType, TestInput)
```

#### **Input**

**ModelOutput**: A list containing the model outputs from fitting the models.

**modelType**: A string characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv', 'senv' and 'xenv'.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta$  on the left. According to different model, it has different size requirement. Default value will be set if the user does not specify.
- TestInput.R: The matrix multiplied to  $\beta$  on the right. According to different model, it has different size requirement. Default value will be set if the user does not specify.
- TestInput.A: The matrix on the right hand side of the equation. Default value will be set if the user does not specify.

#### Output

**TestOutput:** A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of  $vec(L\beta R)$ . A d1 \* d2 by d1 \* d2 matrix.

#### **Description**

This function tests for hypothesis  $H_0: L\beta R = A$ , versus  $H_\alpha: L\beta R \neq A$ . The  $\beta$  is estimated by a model in the envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if  $\beta = 0$  (for 'env', 'ienv', 'penv', 'senv' and 'xenv'), or if the group main effects are all zeros (for 'henv'). The test statistics used is vec  $(L\beta R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom the same as the length of vec(A).

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1:6);
alpha = 0.01;
u = lrt_env(X, Y, alpha);
ModelOutput = env(X, Y, u);
modelType = 'env';
TestOutout = testcoefficient(ModelOutput, modelType);
```

```
Test Hypothesis Chisq Statistic DF P-value L * beta * R = A 116.230 6 0.0000
```

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
Xtemp = fiberpaper(:, 5 : 7);
X.X1 = Xtemp(:, 3);
X.X2 = Xtemp(:, 1 : 2);
alpha = 0.01;
u = lrt_penv(X, Y, alpha);
ModelOutput = penv(X, Y, u);
r = size(Y, 2);
p1 = size(X.X1, 2);
TestInput.L = rand(2, r);
TestInput.R = rand(p1, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_penv(ModelOutput, TestInput);
```

```
Test Hypothesis Chisq Statistic DF P-value

L * beta * R = A 12.598 2 0.0018
```

env

## 2.1 aic\_env

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = aic_env(X, Y)
u = aic_env(X, Y, Opts)
```

#### 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

#### 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.

2.1. AIC\_ENV 23

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

24 CHAPTER 2. ENV

## 2.2 bic\_env

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
u = bic_env(X, Y)
u = bic_env(X, Y, Opts)
```

## 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

#### Output

 $\boldsymbol{u}\!:$  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)
```

2.2. BIC\_ENV 25

u =

1

26 CHAPTER 2. ENV

## 2.3 bstrp\_env

Compute bootstrap standard error for the envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

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

#### 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.

u: Dimension of the envelope subspace. A positive integer between 0 and r.

B: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### 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;
```

2.3. BSTRP\_ENV 27

```
u = lrt_{env}(X, Y, alpha)
u = 1
```

bootse =

- 0.2893
- 0.4260
- 0.3523
- 0.5628
- 0.1675
- 0.6192

28 CHAPTER 2. ENV

## 2.4 dF4env

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

## **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
df = dF4env(R, DataParameter)
```

## Input

**R**: An r by u semi orthogonal matrix, 0 < u < = r.

**DataParameter**: A structure that contains the statistics calculated from the data.

## Output

**df**: An r by u matrix 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.

2.5. ENV 29

## 2.5 env

Fit the envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

## **Syntax**

```
ModelOutput = env(X, Y, u)
ModelOutput = env(X, Y, u, Opts)
```

## **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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the envelope subspace. An r by u matrix. Default value is the one generated by function get\_init.

#### Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- ModelOutput.Sigma: The envelope estimator of the error covariance matrix. An r by r matrix
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. An r by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- ModelOutput.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix.

30 CHAPTER 2. ENV

ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.

- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- ModelOutput.alpha: The estimated intercept in the envelope model. An r by 1 vector.
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of  $vec(\beta)$ . An rp by rp matrix. The covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1/n.
- ModelOutput.asyEnv: The 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/sqrt(n).
- ModelOutput.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.
- ModelOutput.np: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

#### **Description**

This function fits the envelope model to the responses and predictors, using the maximum likelihood 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

- 1. The codes are implemented based on the algorithm in Section 4.3 of Cook et al (2010).
- 2. 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(X, Y, alpha)

u =

ModelOutput = env(X, Y, u)
```

2.5. ENV 31

## ModelOutput =

beta: [6x1 double]
Sigma: [6x6 double]
Gamma: [6x1 double]
Gamma0: [6x5 double]

eta: 8.5647 Omega: 7.8762

OmegaO: [5x5 double] alpha: [6x1 double]

1: -850.7592

covMatrix: [6x6 double]
 asyEnv: [6x1 double]
 ratio: [6x1 double]

np: 28 n: 50

## ModelOutput.Omega

ans =

7.8762

## eig(ModelOutput.Omega0)

ans =

1.0e+03 \*

6.5166

0.2083

0.0201

0.0004

0.0003

## ${\tt ModelOutput.ratio}$

ans =

28.0945

32 CHAPTER 2. ENV

18.4326

23.6384

16.3211

65.8245

6.4668

2.6. F4ENV 33

## 2.6 F4env

Objective function for computing the envelope subspace.

## **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
f = F4env(R, DataParameter)
```

## Input

**R**: An r by u semi orthogonal matrix, 0 < u <= r.

**DataParameter**: A structure that contains the statistics calculated from 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.

34 CHAPTER 2. ENV

## 2.7 lrt\_env

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

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

## 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

## 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 pre-specified significance level  $\alpha$ .

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

2.7. LRT\_ENV 35

u =

1

36 CHAPTER 2. ENV

## 2.8 predict\_env

Perform estimation or prediction under the envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
PredictOutput = predict_env(ModelOutput, Xnew, infType)
```

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from env.

**Xnew**: The value of X with which to estimate or predict Y. A p by 1 vector.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

## Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

#### **Description**

This function evaluates the envelope model at new value Xnew. It can perform estimation: find the fitted value when X = Xnew, or prediction: predict Y when X = Xnew. The covariance matrix and the standard errors are also provided.

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1:6);
alpha = 0.01;
u = lrt_env(X, Y, alpha);
ModelOutput = env(X, Y, u);
Xnew = X(2, :)';
```

PredictOutput = predict\_env(ModelOutput, Xnew, 'estimation')
[PredictOutput.value, Y(1, :)'] % Compare the fitted value with the data
PredictOutput.SE

```
PredictOutput =
        value: [6x1 double]
    covMatrix: [6x6 double]
           SE: [6x1 double]
ans =
  474.7135 468.0000
  127.4740 123.0000
  251.2044 246.0000
  380.8280 374.0000
  380.9473 386.0000
  -6.3287 -11.0000
ans =
    4.8892
    4.0227
    4.3237
    4.7470
    6.8186
    2.6948
       PredictOutput = predict_env(ModelOutput, Xnew, 'prediction')
       PredictOutput.SE
PredictOutput =
        value: [6x1 double]
    covMatrix: [6x6 double]
          SE: [6x1 double]
ans =
  474.7135
  127.4740
  251.2044
  380.8280
  380.9473
  -6.3287
```

38 CHAPTER 2. ENV

ans =

34.9161

28.7280

30.8775

33.9006

48.6945

19.2448

## 2.9 testcoefficient\_env

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\sim$ = A, where beta is estimated under the envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
TestOutput = testcoefficient_env(ModelOutput)
TestOutput = testcoefficient_env(ModelOutput, TestInput)
```

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from env.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta$  on the left. It is a d1 by r matrix, while d1 is less than or equal to r. Default value: identity matrix  $I_r$ .
- TestInput.R: The matrix multiplied to  $\beta$  on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix  $I_p$ .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

#### Output

**TestOutput**: A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of  $vec(L\beta R)$ . A d1 \* d2 by d1 \* d2 matrix.

#### **Description**

This function tests for hypothesis  $H_0: L\beta R = A$ , versus  $H_\alpha: L\beta R \neq A$ . The  $\beta$  is estimated by the envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if  $\beta = 0$ . The test statistics used is vec  $(L\beta R - A)$   $\hat{\Sigma}^{-1}$  vec  $(L\beta R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom d1 \* d2.

40 CHAPTER 2. ENV

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

Test Hypothesis	Chisq Statistic	DF	P-value	
L * beta * R = A	116.230	6	0.0000	

```
r = size(Y, 2);
p = size(X, 2);
TestInput.L = rand(2, r);
TestInput.R = rand(p, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_senv(ModelOutput, TestInput);
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	61.344	2	0.0000

# envpls

## 3.1 bstrp\_envpls

Compute bootstrap standard errors of the envelope model using a sequential algorithm.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
bootse = bstrp_envpls(X, Y, u, B)
bootse = bstrp_envpls(X, Y, u, B, Opts)
```

#### 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 subspace. A positive integer between 0 and p.
- **B**: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameters. If one or several (even all) fields are not defined, the default settings are used.

• Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### Output

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

42 CHAPTER 3. ENVPLS

## Description

This function computes the bootstrap standard errors for the regression coefficients in the envelope model by bootstrapping the residuals. The envelope model is applied for the reduction on X, using a sequential algorithm.

```
load wheatprotein.txt
       X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1 : 6);
       m = 5;
       u = mfoldcv_envpls(X, Y, m)
u =
     0
       B = 100;
       bootse = bstrp_envpls(X, Y, u, B);
bootse =
     0
     0
     0
     0
     0
     0
```

3.2. ENVPLS 43

## 3.2 envpls

Fit the envelope model using a sequential algorithm.

#### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

#### **Syntax**

```
ModelOutput = envpls(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

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

- ModelOutput.beta: The envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- ModelOutput.Sigma: The envelope estimator of the error covariance matrix. An r by r matrix.
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. An r by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- ModelOutput.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- ModelOutput.alpha: The estimated intercept in the envelope model. An r by 1 vector.
- ModelOutput.np: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

44 CHAPTER 3. ENVPLS

#### **Description**

This function fits the envelope model to the responses and predictors, using the maximum likelihood 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 are implemented based on the sequential algorithm in the lecture notes of Cook (2012).

## **Example**

```
load wheatprotein.txt
       X = wheatprotein(:, 8);
       Y = wheatprotein(:, 1 : 6);
       u = mfoldcv_envpls(X, Y, m)
u =
     0
       ModelOutput = envpls(X, Y, u)
ModelOutput =
      beta: [6x1 double]
     Sigma: [6x6 double]
     Gamma: []
    Gamma0: [6x6 double]
       eta: []
     Omega: []
    OmegaO: [6x6 double]
     alpha: [6x1 double]
        np: 27
         n: 50
```

#### ModelOutput.Sigma

```
ans =
  1.0e+03 *
   1.1932 0.9825 1.0568 1.1508
                                  1.5411 0.6340
   0.9825
          0.8222
                  0.8808 0.9391
                                   1.2700
                                         0.5279
```

3.2. ENVPLS 45

1.0568	0.8808	0.9451	1.0125	1.3725	0.5652
1.1508	0.9391	1.0125	1.1239	1.5217	0.6180
1.5411	1.2700	1.3725	1.5217	2.3255	0.8365
0.6340	0.5279	0.5652	0.6180	0.8365	0.3619

46 CHAPTER 3. ENVPLS

## 3.3 mfoldcv\_xenvpls

Select the dimension of the envelope subspace using m-fold cross validation for envelope model on the reduction on X using a sequential algorithm.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = mfoldcv_xenvpls(X, Y, m)
u = mfoldcv_xenvpls(X, Y, m, Opts)
```

#### Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

m: A positive integer that is used to indicate m-fold cross validation.

**Opts**: A list containing the optional input parameters. If one or several (even all) fields are not defined, the default settings are used.

• Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### Output

\*u\*: The dimension of the envelope subspace selected by m-fold cross validation.

### **Description**

This function implements m-fold cross validation to select the dimension of the envelope space, based on prediction performance. For each u, the data is partitioned into m parts, each part is in turn used for testing for the prediction performance while the rest m-1 parts are used for training. The dimension is select as the one that minimizes the average prediction errors. If Y is multivariate, the identity inner product is used for computing the prediction errors.

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

m = 5; u = mfoldcv\_envpls(X, Y, m)

u =

0

## henv

## 4.1 aic henv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = aic_henv(X, Y)
u = aic_henv(X, Y, Opts)
```

#### Input

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

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 greater than p.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0

#### Output

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

4.1. AIC\_HENV 49

## 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)
```

u =

6

## 4.2 bic\_henv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
u = bic_henv(X, Y)
u = bic_henv(X, Y, Opts)
```

#### Input

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

**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 greater than p.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

## 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.

```
load waterstrider.mat
u = bic_henv(X, Y)
```

4.2. BIC\_HENV 51

u =

4

## 4.3 bstrp\_henv

Compute bootstrap standard error for the heteroscedastic envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
bootse = bstrp_henv(X, Y, u, B)
bootse = bstrp_henv(X, Y, u, B, Opts)
```

### Input

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

**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 greater than p.

 $\boldsymbol{u}\text{:}$  Dimension of the envelope subspace. A positive integer between 0 and r.

B: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### 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.

```
load waterstrider.mat
      u = lrt_henv(X, Y, 0.01)
u =
    6
      B = 100;
      bootse = bstrp_henv(X, Y, u, B)
bootse =
   0.0305 0.0466 0.0647
   0.0309 0.0485 0.0682
   0.0305 0.0432
                  0.0638
   0.0205 0.0289 0.0425
   0.0385 0.0553
                  0.0799
   0.0295 0.0427
                    0.0618
   0.0389 0.0567 0.0819
            0.0463
                    0.0665
   0.0321
```

## 4.4 dF4henv

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

#### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
df = dF4henv(R, DataParameter)
```

## Input

**R**: An r by u semi orthogonal matrix, 0 < u <= r.

**DataParameter**: A structure that contains the statistics calculated from the data.

## Output

**df**: An r by u matrix 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.

4.5. F4HENV 55

## 4.5 F4henv

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

#### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
f = F4henv(R, DataParameter)
```

#### Input

**R**: An r by u semi orthogonal matrix, 0 < u <= r.

**DataParameter**: A structure that contains the statistics calculated from 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.

#### 4.6 henv

Fit the heteroscedastic envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

### **Syntax**

```
ModelOutput = henv(X, Y, u)
ModelOutput = henv(X, Y, u, Opts)
```

#### Input

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

**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 greater than p.

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

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the heteroscedastic envelope subspace. An r by u matrix. Default value is the one generated by function get\_init4henv.

### Output

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

- ModelOutput.mu: The heteroscedastic envelope estimator of the grand mean. A r by 1 vector.
- ModelOutput.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.
- ModelOutput.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, ModelOutput.mug alone does not tell which group corresponds to which group mean.

4.6. HENV 57

• ModelOutput.Gamma: The orthogonal basis of the envelope subspace. An r by u semiorthogonal matrix.

- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- ModelOutput.beta: The heteroscedastic envelope estimator of the group main effect. An r by p matrix, the ith column of the matrix contains the main effect for the ith group.
- ModelOutput.groupInd: A matrix containing the unique values of group indicators. The matrix has p rows. The group mean of the ith row is stored in the ith column of ModelOutput.mug.
- ModelOutput.Sigma: The heteroscedastic envelope estimator of the error covariance matrix. A three dimensional matrix with dimension r, r and p, ModelOutput.Sigma(:, :, i) contains the estimated covariance matrix for the ith group.
- ModelOutput.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.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. An u by u by p matrix, ModelOutput.Omega(:, :, i) contains the coordinates of the covariance matrix of the ith group with respect to Gamma.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r u by r u matrix.
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.np: The number of parameters in the heteroscedastic envelope model. A positive integer.
- ModelOutput.covMatrix: The asymptotic covariance of  $(\mu', \text{vec}(\beta'))$ '. An r(p+1) by r(p+1) matrix. The covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1 / n.
- ModelOutput.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).
- ModelOutput.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 ModelOutput.ratio is the elementwise standard error ratio for the ith element in the jth group mean effect.
- ModelOutput.ng: The number of observations in each group. A p by 1 vector.

#### **Description**

This function fits the heteroscedastic envelope model to the responses and predictors, using the maximum likelihood 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

- 1. The codes are implemented based on the algorithm in Section 2.2 of Su and Cook (2012).
- 2. 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 water strider example in Su and Cook (2011).

```
load waterstrider.mat
      u = lrt_henv(X, Y, 0.01)
u =
    6
      ModelOutput = henv(X, Y, u)
      ModelOutput.ratio
ModelOutput =
          mu: [8x1 double]
         mug: [8x3 double]
        Yfit: [90x8 double]
       Gamma: [8x6 double]
      Gamma0: [8x2 double]
        beta: [8x3 double]
    groupInd: [3x2 double]
       Sigma: [8x8x3 double]
         eta: [6x3 double]
       Omega: [6x6x3 double]
      OmegaO: [2x2 double]
          np: 98
           1: 1.0051e+03
    covMatrix: [32x32 double]
     asyHenv: [8x3 double]
       ratio: [8x3 double]
          ng: [3x1 double]
ans =
   6.5439 11.2830 6.4954
   4.6325 5.3226
                      4.7242
           5.0741
   4.4456
                      4.4198
   4.7338
           6.2469 5.1937
                    9.4823
   8.0377
           12.5386
   9.5067 11.5974 11.3444
   11.8632
           15.6080 12.5611
   6.9792 11.1559 10.1002
```

4.7. LRT\_HENV 59

## 4.7 lrt\_henv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
u = lrt_henv(X, Y, alpha)
u = lrt_henv(X, Y, alpha, Opts)
```

### Input

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

**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 greater than p.

alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

### 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 pre-specified significance level  $\alpha$ .

## Example

```
load waterstrider.mat
u = lrt_henv(X, Y, 0.01)
```

u =

6

## 4.8 predict\_henv

Perform estimation or prediction under the heteroscedastic envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
PredictOutput = predict_henv(ModelOutput, Xnew, infType)
```

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from henv.

**Xnew**: A group indicator. It must be a column vector, whose transpose is the same as one of the group indictors from the original data.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

#### Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix.
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

#### **Description**

This function evaluates the inner envelope model at new value Xnew. It can perform estimation: find the group mean for the group indicated by Xnew, or prediction: predict Y for the group indicated by Xnew. The covariance matrix and the standard errors are also provided.

```
load waterstrider.mat
u = lrt_henv(X, Y, 0.01);
ModelOutput = henv(X, Y, u);
ModelOutput.groupInd
ModelOutput.mug
Xnew = X(1, :)'
```

```
ans =
   -1
         -1
    0
          1
          0
    1
ans =
  -1.1417 -1.1267 -1.0845
            -1.4067 -1.3132
   -1.4063
  -1.3314 -1.3336 -1.2152
   -0.3113
           -0.1839 -0.1736
   0.4003 0.3847 0.3072
   0.4107 0.3753 0.3735
          0.3271
   0.3467
                    0.3179
   -0.1954 \quad -0.2100 \quad -0.3488
Xnew =
    1
    0
      PredictOutput = predict_henv(ModelOutput, Xnew, 'estimation')
      PredictOutput.value %This is the 3rd group mean
      PredictOutput.SE
PredictOutput =
       value: [8x1 double]
   covMatrix: [8x8 double]
          SE: [8x1 double]
ans =
  -1.0845
  -1.3132
  -1.2152
  -0.1736
   0.3072
   0.3735
   0.3179
   -0.3488
```

0.3854

```
ans =
    0.0682
    0.0695
    0.0651
    0.0436
    0.0832
    0.0636
    0.0847
    0.0698
       PredictOutput = predict_henv(ModelOutput, Xnew, 'prediction')
       PredictOutput.SE
PredictOutput =
        value: [8x1 double]
    covMatrix: [8x8 double]
           SE: [8x1 double]
ans =
    0.3720
    0.3812
    0.3581
    0.2398
    0.4612
    0.3519
    0.4710
```

## 4.9 testcoefficient\_henv

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\sim$ = A, where beta is estimated under the heteroscedastic envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
TestOutput = testcoefficient_henv(ModelOutput)
TestOutput = testcoefficient_henv(ModelOutput, TestInput)
```

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from henv.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta$  on the left. It is a d1 by r matrix, while d1 is less than or equal to r 1. Default value: identity matrix  $I_r$ .
- TestInput.R: The matrix multiplied to  $\beta$  on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix  $(I_{p-1}, 0_{(p-1)\times 1})^T$ . This is because the columns of  $\beta$  sum to 0. Then we cannot use  $I_p$  as default.
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

#### Output

**TestOutput**: A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of  $vec(L\beta R)$ . A d1 \* d2 by d1 \* d2 matrix.

## Description

This function tests for hypothesis  $H_0: L\beta R = A$ , versus  $H_\alpha: L\beta R \neq A$ . The  $\beta$  is estimated by the heteroscedastic envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if all the main group effects are 0. The test

statistics used is vec  $(L\beta R - A)$   $\hat{\Sigma}^{-1}$  vec  $(L\beta R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom d1 \* d2.

```
load waterstrider.mat
u = lrt_henv(X, Y, 0.01);
ModelOutput = henv(X, Y, u);
TestOutout = testcoefficient_henv(ModelOutput);
```

Test Hypothesis	Chisq Statistic	DF	P-value	
L * beta * R = A	226.256	16	0.0000	

```
r = size(Y, 2);
p = size(ModelOutput.beta, 2);
TestInput.L = rand(2, r);
TestInput.R = rand(p, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_henv(ModelOutput, TestInput);
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	23.429	2	0.0000

## ienv

## 5.1 aic\_ienv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = aic_ienv(X, Y)
u = aic_ienv(X, Y, Opts)
```

#### 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- $\bullet\,$  Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

#### Output

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

5.1. AIC\_IENV 67

## Description

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

```
load irisf.mat
u = aic_ienv(X, Y)

u =
```

68 CHAPTER 5. IENV

## 5.2 bic\_ienv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
u = bic_ienv(X, Y)
u = bic_ienv(X, Y, Opts)
```

#### 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

#### 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.

```
load irisf.mat
u = bic_ienv(X, Y)
u =
```

5.3. BSTRP\_IENV 69

## 5.3 bstrp\_ienv

Compute bootstrap standard error for the inner envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
bootse = bstrp_ienv(X, Y, u, B)
bootse = bstrp_ienv(X, Y, u, B, Opts)
```

#### 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.

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

**B**: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### 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
u = bic_ienv(X, Y)
```

70 CHAPTER 5. IENV

```
u =
    1

B = 100;
bootse = bstrp_ienv(X, Y, u, B)

bootse =
    13.4695     4.9601
    7.4709     2.7315
```

14.9316 5.2913 8.7597 3.0853 5.4. DF4IENV 71

## 5.4 dF4ienv

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

#### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
df = dF4ienv(R, DataParameter)
```

## Input

**R**: An r by u semi-orthogonal matrix, 0 < u <= p.

**DataParameter**: A structure that contains the statistics calculated from 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.

72 CHAPTER 5. IENV

## 5.5 F4ienv

Objective function for computing the inner envelope subspace.

#### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
f = F4ienv(R, DataParameter)
```

#### Input

**R**: An r by u semi orthogonal matrix, 0 < u <= p.

**DataParameter**: A structure that contains the statistics calculated from 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.

5.6. IENV 73

#### **5.6** ienv

Fit the inner envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

#### **Syntax**

```
ModelOutput = ienv(X, Y, u)
ModelOutput = ienv(X, Y, u, Opts)
```

#### 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the inner envelope subspace. An r by u matrix. Default value is the one generated by function get\_init.

#### Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- ModelOutput.Sigma: The envelope estimator of the error covariance matrix. An r by r matrix.
- ModelOutput.Gamma1: The orthogonal basis of the inner envelope subspace. An r by u semi-orthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the inner envelope subspace. An r by r-u semi-orthogonal matrix.

74 CHAPTER 5. IENV

• ModelOutput.eta1: The transpose of the coordinates of  $\beta$  with respect to Gamma1. An p by u matrix.

- ModelOutput.B: An (r u) by (p u) semi-orthogonal matrix, so that (Gamma, Gamma0 \* B) spans  $\beta$ .
- ModelOutput.eta2: The transpose of the coordinates of  $\beta$  with respect to Gamma0. An p by (p-u) matrix.
- ModelOutput.Omega1: The coordinates of Sigma with respect to Gamma1. An u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r u by r - u matrix.
- ModelOutput.alpha: The estimated intercept in the inner envelope model. An r by 1 vector.
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of  $vec(\beta)$ . An rp by rp matrix. The covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1/n.
- ModelOutput.asyIenv: 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 / sqrt(n).
- ModelOutput.ratio: The asymptotic standard error ratio of the standard multivariate linear regression estimator over the inner envelope estimator, for each element in  $\beta$ . An r by p matrix.
- ModelOutput.np: The number of parameters in the inner envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

### **Description**

This function fits the inner envelope model to the responses and predictors, using the maximum likelihood 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

- 1. The codes are implemented based on the algorithm in Su and Cook (2012).
- 2. 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**

1

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

```
load irisf.mat

d = bic_ienv(X, Y)

d =
```

5.6. IENV 75

# ModelOutput = ienv(X, Y, d) 1 - 1 ./ ModelOutput.ratio

### ModelOutput =

beta: [4x2 double] Sigma: [4x4 double] Gamma1: [4x1 double] Gamma0: [4x3 double] B: [3x1 double] eta1: [2x1 double] eta2: [2x1 double] Omega1: 8.3751 Omega0: [3x3 double] alpha: [4x1 double] np: 16 1: -1.4805e+03 covMatrix: [8x8 double] asyIenv: [4x2 double] ratio: [4x2 double] n: 150

ans =

0.0049 0.2122 0.0020 0.0806 0.0033 0.1404 0.0004 0.0138 76 CHAPTER 5. IENV

## 5.7 lrt\_ienv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = lrt_ienv(X, Y, alpha)
u = lrt_ienv(X, Y, alpha, Opts)
```

#### 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

## Output

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 pre-specified significance level  $\alpha$ .

```
load irisf.mat
alpha = 0.01;
u = lrt_ienv(X, Y, alpha)
```

5.7. LRT\_IENV 77

u =

1

78 CHAPTER 5. IENV

## 5.8 predict\_ienv

Perform estimation or prediction under the inner envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
PredictOutput = predict_ienv(ModelOutput, Xnew, infType)
```

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from ienv.

**Xnew**: The value of X with which to estimate or predict Y. A p by 1 vector.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

### Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix.
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

#### **Description**

This function evaluates the inner envelope model at new value Xnew. It can perform estimation: find the fitted value when X = Xnew, or prediction: predict Y when X = Xnew. The covariance matrix and the standard errors are also provided.

```
load irisf.mat
d = bic_ienv(X, Y);
ModelOutput = ienv(X, Y, d);
Xnew = X(1, :)';
PredictOutput = predict_ienv(ModelOutput, Xnew, 'estimation')
[PredictOutput.value, Y(1, :)'] % Compare the fitted value with the data
PredictOutput.SE
```

2.0642

```
PredictOutput =
       value: [4x1 double]
   covMatrix: [4x4 double]
          SE: [4x1 double]
ans =
  49.9458 51.0000
  34.2592 35.0000
  14.5771 14.0000
   2.4513 2.0000
ans =
   1.0978
   0.7146
   0.9265
   0.4357
      PredictOutput = predict_ienv(ModelOutput, Xnew, 'prediction')
      PredictOutput.SE
PredictOutput =
       value: [4x1 double]
    covMatrix: [4x4 double]
         SE: [4x1 double]
ans =
   5.2197
   3.3897
   4.3996
```

80 CHAPTER 5. IENV

## 5.9 testcoefficient\_ienv

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\sim$ = A, where beta is estimated under the inner envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
TestOutput = testcoefficient_ienv(ModelOutput)
TestOutput = testcoefficient_ienv(ModelOutput, TestInput)
```

## Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from ienv.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta$  on the left. It is a d1 by r matrix, while d1 is less than or equal to r. Default value: identity matrix  $I_r$ .
- TestInput.R: The matrix multiplied to  $\beta$  on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix  $I_p$ .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

### Output

**TestOutput**: A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of  $vec(L\beta R)$ . A d1 \* d2 by d1 \* d2 matrix.

#### **Description**

This function tests for hypothesis  $H_0: L\beta R = A$ , versus  $H_\alpha: L\beta R \neq A$ . The  $\beta$  is estimated by the inner envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if  $\beta = 0$ . The test statistics used is vec  $(L\beta R - A)$   $\hat{\Sigma}^{-1}$  vec  $(L\beta R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom d1 \* d2.

```
load irisf.mat
d = bic_ienv(X,Y);
ModelOutput = ienv(X,Y,d);
TestOutout = testcoefficient_ienv(ModelOutput);
```

Test Hypothesis	Chisq Statistic	DF	P-value		
L * beta * R = A	4642.913	8	0.0000		

```
TestInput.L = rand(2, 4);
TestInput.R = rand(2, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_ienv(ModelOutput, TestInput);
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	1834.229	2	0.0000

## penv

## 6.1 aic\_penv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = aic_penv(X, Y)
u = aic_penv(X, Y, Opts)
```

#### Input

**X**: A list containing the value of X1 and X2.

- X.X1: Predictors of main interest. 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.
- X.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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

### Output

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

6.1. AIC\_PENV 83

## Description

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

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
Xtemp = fiberpaper(:, 5 : 7);
X.X1 = Xtemp(:, 3);
X.X2 = Xtemp(:, 1 : 2);
u = aic_penv(X, Y)
```

## 6.2 bic\_penv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = bic_penv(X, Y)
u = bic_penv(X, Y, Opts)
```

#### Input

**X**: A list containing the value of X1 and X2.

- X.X1: Predictors of main interest. 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.
- X.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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

### Output

 $\boldsymbol{u}\!:$  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.

6.2. BIC\_PENV 85

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
Xtemp = fiberpaper(:, 5 : 7);
X.X1 = Xtemp(:, 3);
X.X2 = Xtemp(:, 1 : 2);
u = bic_penv(X, Y)
```

## 6.3 bstrp\_penv

Compute bootstrap standard error for the partial envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
bootse = bstrp_penv(X, Y, u, B)
bootse = bstrp_penv(X, Y, u, B, Opts)
```

#### Input

**X**: A list containing the value of X1 and X2.

- X.X1: Predictors of main interest. 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.
- X.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.

- u: Dimension of the partial envelope subspace. A positive integer between 0 and r.
- **B**: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

#### 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 fiberpaper.dat
       Y = fiberpaper(:, 1 : 4);
       Xtemp = fiberpaper(:, 5 : 7);
       X.X1 = Xtemp(:, 3);
       X.X2 = Xtemp(:, 1 : 2);
       alpha = 0.01;
       u = lrt_penv(X, Y, alpha)
u =
    1
       B = 100;
       bootse = bstrp_penv(X, Y, u, B)
bootse =
    0.0074
    0.0021
    0.0043
    0.0019
```

## 6.4 lrt\_penv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
u = lrt_penv(X, Y, alpha)
u = lrt_penv(X, Y, alpha, Opts)
```

#### Input

**X**: A list containing the value of X1 and X2.

- X.X1: Predictors of main interest. 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.
- X.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.

alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value:
   0.

#### Output

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 pre-specified significance level  $\alpha$ .

6.4. LRT\_PENV 89

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
Xtemp = fiberpaper(:, 5 : 7);
X.X1 = Xtemp(:, 3);
X.X2 = Xtemp(:, 1 : 2);
alpha = 0.01;
u = lrt_penv(X, Y, alpha)
u =
```

## 6.5 penv

Fit the partial envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

## **Syntax**

```
ModelOutput = penv(X, Y, u)
ModelOutput = penv(X, Y, u, Opts)
```

#### Input

**X**: A list containing the value of X1 and X2.

- X.X1: Predictors of main interest. 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.
- X.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, and r should be strictly greater than p1.

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

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the partial envelope subspace. An r by u matrix. Default value is the one generated by function get\_init.

#### Output

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

- ModelOutput.beta1: The partial envelope estimator of  $\beta_1$ , which is the regression coefficients for X1. An r by p1 matrix.
- ModelOutput.beta2: The partial envelope estimator of  $\beta_2$ , which is the regression coefficients for X2. An r by p2 matrix.

6.5. PENV 91

• ModelOutput.Sigma: The partial envelope estimator of the error covariance matrix. An r by r matrix.

- ModelOutput.Gamma: The orthogonal basis of the partial envelope subspace. An r by u semi-orthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the partial envelope subspace. An r by r u semi-orthogonal matrix.
- Model Output.eta: The coordinates of  $\beta_1$  with respect to Gamma. An u by p1 matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r u by r

   u matrix.
- ModelOutput.alpha: The estimated intercept in the partial envelope model. An r by 1 vector
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of  $(\text{vec}(\beta_2)', \text{vec}(\beta_1)')$ . An rp by rp matrix. The covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1/n.
- ModelOutput.asyPenv: Asymptotic standard error for elements in  $\beta_1$  under the partial envelope model. An r by p1 matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by 1/sqrt(n).
- ModelOutput.ratio: The asymptotic standard error ratio of the standard multivariate linear regression estimator over the partial envelope estimator, for each element in  $\beta_1$ . An r by p1 matrix.
- ModelOutput.np: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

## Description

This function fits the partial envelope model to the responses Y and predictors X1 and X2, using the maximum likelihood 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

- 1. The codes are implemented based on the algorithm in Section 3.2 of Su and Cook (2012).
- 2. 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).

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
Xtemp = fiberpaper(:, 5 : 7);
X.X1 = Xtemp(:, 3);
X.X2 = Xtemp(:, 1 : 2);
```

```
alpha = 0.01;
       u = lrt_penv(X, Y, alpha)
u =
     1
       ModelOutput = penv(X, Y, u)
       ModelOutput.Omega
       eig(ModelOutput.Omega0)
       ModelOutput.ratio
ModelOutput =
        beta1: [4x1 double]
        beta2: [4x2 double]
        alpha: [4x1 double]
        Gamma: [4x1 double]
          eta: 0.0047
        Omega: 0.0149
       Omega0: [3x3 double]
        Sigma: [4x4 double]
            1: -35.6323
           np: 23
    covMatrix: [12x12 double]
      asyPenv: [4x1 double]
        ratio: [4x1 double]
           n: 62
ans =
    0.0149
ans =
    4.9819
    0.0999
    0.0050
ans =
   66.0742
   6.9326
   10.5048
    9.6279
```

## 6.6 predict\_penv

Perform estimation or prediction under the partial envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

PredictOutput = predict\_penv(ModelOutput, Xnew, infType)

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from penv.

Xnew: A list containing the value of X1 and X2 with which to estimate or predict Y.

```
* Xnew.X1: A p1 by 1 vector containing the value of X1.
```

\* Xnew.X2: A p2 by 1 vector containing the value of X2.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

## Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix.
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

## **Description**

This function evaluates the envelope model at new value Xnew. It can perform estimation: find the fitted value when X = Xnew, or prediction: predict Y when X = Xnew. The covariance matrix and the standard errors are also provided.

```
load fiberpaper.dat
       Y = fiberpaper(:, 1 : 4);
      Xtemp = fiberpaper(:, 5 : 7);
       X.X1 = Xtemp(:, 3);
      X.X2 = Xtemp(:, 1 : 2);
       alpha = 0.01;
       u = lrt_penv(X, Y, alpha);
       ModelOutput = penv(X, Y, u);
       Xnew.X1 = X.X1(1, :)';
       Xnew.X2 = X.X2(1, :)';
       PredictOutput = predict_penv(ModelOutput, Xnew, 'estimation')
       [PredictOutput.value, Y(1, :)'] % Compare the fitted value with the data
       PredictOutput.SE
PredictOutput =
       value: [4x1 double]
    covMatrix: [4x4 double]
          SE: [4x1 double]
ans =
   21.1169 21.3120
   7.1173 7.0390
   5.3637
             5.3260
   0.8737 0.9320
ans =
   1.4680
   0.4234
   0.7145
   0.3161
       PredictOutput = predict_penv(ModelOutput, Xnew, 'prediction')
       PredictOutput.SE
PredictOutput =
       value: [4x1 double]
    covMatrix: [4x4 double]
          SE: [4x1 double]
ans =
```

- 2.4277
- 0.6982
- 1.1802
- 0.5220

## 6.7 testcoefficient\_penv

This function tests the null hypothesis L \* beta1 \* R = A versus the alternative hypothesis L \* beta1 \* R  $\sim$ = A, where beta1 is estimated under the envelope model.

## **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
TestOutput = testcoefficient_penv(ModelOutput)
TestOutput = testcoefficient_penv(ModelOutput, TestInput)
```

## Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from penv.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta_1$  on the left. It is a d1 by r matrix, while d1 is less than or equal to r. Default value: identity matrix  $I_r$ .
- TestInput.R: The matrix multiplied to  $\beta_1$  on the right. It is a p1 by d2 matrix, while d2 is less than or equal to p1. Default value: identity matrix  $I_{p1}$ .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

### Output

**TestOutput**: A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of vec( $L\beta_1R$ ). A d1 \* d2 by d1 \* d2 matrix.

#### **Description**

This function tests for hypothesis  $H_0: L\beta_1R = A$ , versus  $H_\alpha: L\beta_1R \neq A$ . The  $\beta_1$  is estimated by the partial envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if  $\beta_1 = 0$ . The test statistics used is vec  $(L\beta_1R - A)$   $\hat{\Sigma}^{-1}$  vec  $(L\beta_1R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom d1 \* d2.

```
load fiberpaper.dat
     Y = fiberpaper(:, 1 : 4);
     Xtemp = fiberpaper(:, 5 : 7);
     X.X1 = Xtemp(:, 3);
     X.X2 = Xtemp(:, 1 : 2);
     alpha = 0.01;
     u = lrt_penv(X, Y, alpha);
     ModelOutput = penv(X, Y, u);
     TestOutout = testcoefficient_penv(ModelOutput);
Test Hypothesis Chisq Statistic DF P-value
______
L * beta * R = A 12.604 4 0.0134
     r = size(Y, 2);
     p1 = size(X.X1, 2);
     TestInput.L = rand(2, r);
     TestInput.R = rand(p1, 1);
     TestInput.A = zeros(2, 1);
     TestOutout = testcoefficient_penv(ModelOutput, TestInput);
Test Hypothesis Chisq Statistic DF P-value
______
L * beta * R = A 11.452 2 0.0033
```

## senv

## 7.1 aic\_senv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
u = aic_senv(X, Y)
u = aic_senv(X, Y, Opts)
```

#### 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

#### 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.

7.1. AIC\_SENV 99

```
load('sales.txt')
Y = sales(:, 4 : 7);
X = sales(:, 1 : 3);
u = aic_senv(X, Y)
```

100 CHAPTER 7. SENV

## 7.2 bic\_senv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
u = bic_senv(X, Y)
u = bic_senv(X, Y, Opts)
```

## 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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

#### Output

 $\boldsymbol{u}\text{:}$  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.

```
load('sales.txt')
Y = sales(:, 4 : 7);
X = sales(:, 1 : 3);
u = bic_senv(X, Y)
```

7.2. BIC\_SENV 101

u =

2

102 CHAPTER 7. SENV

## 7.3 bstrp\_senv

Compute bootstrap standard error for the scaled envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
bootse = bstrp_senv(X, Y, u, B)
bootse = bstrp_senv(X, Y, u, B, Opts)
```

#### 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.

u: Dimension of the envelope subspace. A positive integer between 0 and r.

**B**: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

### 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.

```
load('sales.txt')
Y = sales(:, 4 : 7);
X = sales(:, 1 : 3);
```

7.3. BSTRP\_SENV 103

```
u = bic_senv(X, Y)

u =

2

B = 20;
bootse = bstrp_senv(X, Y, u, B)
```

0.0539 0.0472 0.0554

0.06750.09120.11780.05670.07810.07910.09860.09440.1283

104 CHAPTER 7. SENV

## 7.4 dF4senv

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

#### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
df = dF4senv(R, DataParameter)
```

## Input

**R**: An r by u semi-orthogonal matrix, 0 < u <= r.

**DataParameter**: A structure that contains the statistics calculated from 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.

7.5. F4SENV 105

### **7.5** F4senv

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

### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
f = F4senv(R, DataParameter)
```

## Input

**R**: An r by u semi orthogonal matrix, 0 < u <= r.

**DataParameter**: A structure that contains the statistics calculated from 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.

106 CHAPTER 7. SENV

## 7.6 objfun

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

### **Contents**

- Syntax
- Input
- Output
- Description

## **Syntax**

```
f = objfun(d, Gamma, DataParameter)
```

## Input

 ${f d}$ : 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-orthogonal 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.

## 7.7 predict\_senv

Perform estimation or prediction under the scaled envelope model.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
PredictOutput = predict_senv(ModelOutput, Xnew, infType)
```

#### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from senv.

**Xnew**: The value of X with which to estimate or predict Y. A p by 1 vector.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

### Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

#### **Description**

This function evaluates the scaled envelope model at new value Xnew. It can perform estimation: find the fitted value when X = Xnew, or prediction: predict Y when X = Xnew. The covariance matrix and the standard errors are also provided.

```
load('sales.txt')
Y = sales(:, 4 : 7);
X = sales(:, 1 : 3);
u = bic_senv(X, Y);
ModelOutput = senv(X, Y, u);
Xnew = X(1, :)';
PredictOutput = predict_senv(ModelOutput, Xnew, 'estimation')
```

108 CHAPTER 7. SENV

[PredictOutput.value, Y(1, :)'] % Compare the fitted value with the data PredictOutput.SE

```
PredictOutput =
       value: [4x1 double]
    covMatrix: [4x4 double]
          SE: [4x1 double]
ans =
   8.9109 9.0000
   11.5096 12.0000
   9.6063 9.0000
   19.5119 20.0000
ans =
   7.7627
   5.8952
   4.2205
    8.0134
       PredictOutput = predict_senv(ModelOutput, Xnew, 'prediction')
      PredictOutput.SE
PredictOutput =
       value: [4x1 double]
    covMatrix: [4x4 double]
          SE: [4x1 double]
ans =
   8.3024
   6.3052
    4.4254
    8.5956
```

7.8. SENV 109

### **7.8** senv

Fit the scaled envelope model.

#### **Contents**

- Svntax
- Input
- Output
- Description
- References
- Example

### **Syntax**

```
ModelOutput = senv(X, Y, u)
ModelOutput = senv(X, Y, u, Opts)
```

### **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.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out number of iterations, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the envelope subspace. An r by u matrix. Default value is the one generated by function get\_init.

### Output

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

- ModelOutput.beta: The scaled envelope estimator of the regression coefficients  $\beta$ . An r by p matrix.
- ModelOutput.Sigma: The scaled envelope estimator of the error covariance matrix. An r by r matrix.
- ModelOutput.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.
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. An r by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r u semi-orthogonal matrix.

110 CHAPTER 7. SENV

- ModelOutput.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. An u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r u by r

   u matrix.
- ModelOutput.alpha: The estimated intercept in the scaled envelope model. An r by 1 vector.
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of vec(β). An rp by rp matrix. The
  covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1
  / n.
- ModelOutput.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 / sqrt(n).
- ModelOutput.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.
- ModelOutput.np: The number of parameters in the scaled envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

### **Description**

This function fits the scaled envelope model to the responses and predictors, using the maximum likelihood 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 r and r are uncorrelated, and the fitting is different.

#### References

- 1. The codes are implemented based on the algorithm in Section 4.1 of Cook and Su (2012).
- 2. 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('sales.txt')
Y = sales(:, 4 : 7);
X = sales(:, 1 : 3);
u = bic_senv(X, Y)
```

u =

7.8. SENV

# ModelOutput = senv(X, Y, u) ModelOutput.Lambda 1 - 1 ./ ModelOutput.ratio

### ModelOutput =

beta: [4x3 double]
Sigma: [4x4 double]
Lambda: [4x4 double]
Gamma: [4x2 double]
GammaO: [4x2 double]
eta: [2x3 double]
Omega: [2x2 double]
OmegaO: [2x2 double]
alpha: [4x1 double]
np: 23
1: -386.1900

covMatrix: [12x12 double] asySenv: [4x3 double]

ratio: [4x3 double]

n: 50

ans =

0	0	0	1.0000
0	0	0.9729	0
0	0.8067	0	0
1.7016	0	0	0

ans =

0.7020	0.5218	0.6517
0.6137	0.3219	0.5614
0.4439	0.1858	0.3924
0.5375	0.4639	0.5228

112 CHAPTER 7. SENV

# 7.9 testcoefficient\_senv

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\sim$ = A, where beta is estimated under the scaled envelope model.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
TestOutput = testcoefficient_senv(ModelOutput)
TestOutput = testcoefficient_senv(ModelOutput, TestInput)
```

### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from senv.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta$  on the left. It is a d1 by r matrix, while d1 is less than or equal to r. Default value: identity matrix  $I_r$ .
- TestInput.R: The matrix multiplied to  $\beta$  on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix  $I_p$ .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

### Output

**TestOutput**: A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of  $vec(L\beta R)$ . A d1 \* d2 by d1 \* d2 matrix.

### **Description**

This function tests for hypothesis  $H_0: L\beta R = A$ , versus  $H_\alpha: L\beta R \neq A$ . The  $\beta$  is estimated by the scaled envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if  $\beta = 0$ . The test statistics used is vec  $(L\beta R - A)$   $\hat{\Sigma}^{-1}$  vec  $(L\beta R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom d1 \* d2.

```
load('sales.txt')
Y = sales(:,4:7);
X = sales(:,1:3);
u = bic_senv(X,Y)
ModelOutput = senv(X,Y,u);
TestOutout = testcoefficient_senv(ModelOutput);
```

Test Hypothesis	Chisq Statistic	DF	P-value	
L * beta * R = A	4827.816	12	0.0000	

```
r = size(Y, 2);
p = size(X, 2);
TestInput.L = rand(2, r);
TestInput.R = rand(p, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_senv(ModelOutput, TestInput);
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	1025.948	 2	0.0000
L * Deta * K - A	1023.940	_	0.0000

# xenv

# 8.1 aic\_xenv

Use Akaike information criterion to select the dimension of the envelope subspace for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = aic_xenv(X, Y)
u = aic_xenv(X, Y, Opts)
```

### **Input**

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

### Output

 ${f u}$ : Dimension of the envelope. An integer between 0 and p.

8.1. AIC\_XENV 115

# Description

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

```
load wheatprotein.txt
X = wheatprotein(:, 1 : 6);
Y = wheatprotein(:, 7);
u = aic_xenv(X, Y)
```

116 CHAPTER 8. XENV

# 8.2 bic\_xenv

Use Bayesian information criterion to select the dimension of the envelope subspace for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = bic_xenv(X, Y)
u = bic_xenv(X, Y, Opts)
```

### Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

### Output

**u**: Dimension of the envelope. An integer between 0 and p.

### **Description**

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

```
load wheatprotein.txt
X = wheatprotein(:, 1 : 6);
Y = wheatprotein(:, 7);
u = bic_xenv(X, Y)
```

8.2. BIC\_XENV 117

u =

4

118 CHAPTER 8. XENV

# 8.3 bstrp\_xenv

Compute bootstrap standard error of the envelope model for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
bootse = bstrp_xenv(X, Y, u, B)
bootse = bstrp_xenv(X, Y, u, B, Opts)
```

### Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

**u**: Dimension of the envelope subspace. A positive integer between 0 and p.

**B**: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

### Output

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

### **Description**

This function computes the bootstrap standard errors for the regression coefficients in the envelope model by bootstrapping the residuals. The envelope model here is for the reduction on X.

```
load wheatprotein.txt
       X = wheatprotein(:, 1 : 6);
       Y = wheatprotein(:, 7);
       alpha = 0.01;
       u = lrt\_xenv(X, Y, alpha)
u =
     4
       B = 100;
       bootse = bstrp_xenv(X, Y, u, B)
bootse =
    0.0222
    0.0387
    0.0413
    0.0167
    0.0022
    0.0087
```

120 CHAPTER 8. XENV

# 8.4 dF4xenv

The first derivative of the objective function for computing the envelope subspace for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description

# **Syntax**

```
df = dF4xenv(R, DataParameter)
```

# Input

**R**: A p by u semi orthogonal matrix, 0 < u <= p.

**DataParameter**: A structure that contains the statistics calculated from the data.

# Output

**df**: An p by u matrix containing the value of the derivative function evaluated at R.

# **Description**

The objective function is derived in Section 4.5.1 of Cook et al. (2012) by using maximum likelihood estimation. This function is the derivative of the objective function.

8.5. F4XENV 121

### 8.5 F4xenv

Objective function for computing the envelope subspace for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description

# **Syntax**

```
f = F4xenv(R, DataParameter)
```

# Input

**R**: A p by u semi orthogonal matrix, 0 < u <= p.

**DataParameter**: A structure that contains the statistics calculated from the data.

# Output

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

# **Description**

The objective function is derived in Section 4.5.1 of Cook et al. (2012) using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace.

122 CHAPTER 8. XENV

# 8.6 lrt\_xenv

Use likelihood ratio testing to select the dimension of the envelope subspace for the reduction on X.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = lrt_xenv(X, Y, alpha)
u = lrt_xenv(X, Y, alpha, Opts)
```

### Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out dimension selection process, logical 0 or 1. Default value: 0.

### Output

**u**: Dimension of the envelope. An integer between 0 and p.

### **Description**

This function implements the likelihood ratio testing procedure to select the dimension of the envelope subspace for the reduction on X, with pre-specified significance level  $\alpha$ .

8.6. LRT\_XENV 123

```
load wheatprotein.txt
X = wheatprotein(:, 1 : 6);
Y = wheatprotein(:, 7);
alpha = 0.01;
u = lrt_xenv(X, Y, alpha)
```

124 CHAPTER 8. XENV

# 8.7 predict\_xenv

Perform estimation or prediction under the envelope model for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
PredictOutput = predict_xenv(ModelOutput, Xnew, infType)
```

### Input

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from xenv.

**Xnew**: The value of X with which to estimate or predict Y. A p by 1 vector.

**infType**: A string of characters indicting the inference type, the choices can be 'estimation' or 'prediction'.

### Output

**PredictOutput**: A list containing the results of the inference.

- PredictOutput.value: The fitted value or the prediction value evaluated at Xnew. An r by 1 vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. An r by r matrix
- PredictOutput.SE: The standard error of elements in PredictOutput.value. An r by 1 vector.

### **Description**

This function evaluates the envelope model for the reduction on X at new value Xnew. It can perform estimation: find the fitted value when X = Xnew, or prediction: predict Y when X = Xnew. The covariance matrix and the standard errors are also provided.

```
load wheatprotein.txt
X = wheatprotein(:, 1 : 6);
Y = wheatprotein(:, 7);
u = bic_xenv(X, Y)
ModelOutput = xenv(X, Y, u);
Xnew = X(1, :)';
PredictOutput = predict_xenv(ModelOutput, Xnew, 'estimation')
```

[PredictOutput.value, Y(1, :)']  $\,\,\%$  Compare the fitted value with the data PredictOutput.SE

```
PredictOutput =
       value: 9.1751
   covMatrix: 16.8439
          SE: 4.1041
ans =
   9.1751 9.2300
ans =
   4.1041
      PredictOutput = predict_xenv(ModelOutput, Xnew, 'prediction')
      PredictOutput.SE
PredictOutput =
       value: 9.1751
    covMatrix: 16.8760
         SE: 4.1080
ans =
   4.1080
```

126 CHAPTER 8. XENV

### 8.8 testcoefficient xenv

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\sim$ = A, where beta is estimated under the envelope model for the reduction on X.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

# **Syntax**

```
TestOutput = testcoefficient_xenv(ModelOutput)
TestOutput = testcoefficient_xenv(ModelOutput, TestInput)
```

### **Input**

**ModelOutput**: A list containing the maximum likelihood estimators and other statistics inherited from xenv.

**TestInput**: A list that specifies the null hypothesis, including L, R, and A. If not provided by the user, default values will be used.

- TestInput.L: The matrix multiplied to  $\beta$  on the left. It is a d1 by p matrix, while d1 is less than or equal to p. Default value: identity matrix  $I_p$ .
- TestInput.R: The matrix multiplied to  $\beta$  on the right. It is a r by d2 matrix, while d2 is less than or equal to r. Default value: identity matrix  $I_r$ .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

### Output

**TestOutput**: A list containing test statistics, degrees of freedom for the reference chi-squared distribution, the p-value, and the covariance matrix of  $vec(L\beta R)$ . At the same time, a table is printed out.

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of  $vec(L\beta R)$ . A d1 \* d2 by d1 \* d2 matrix.

### **Description**

This function tests for hypothesis  $H_0: L\beta R = A$ , versus  $H_\alpha: L\beta R \neq A$ . The  $\beta$  is estimated by the envelope model for the reduction on X. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if  $\beta = 0$ . The test statistics used is vec  $(L\beta R - A)$   $\hat{\Sigma}^{-1}$  vec  $(L\beta R - A)^T$ , and the reference distribution is chi-squared distribution with degrees of freedom d1 \* d2.

```
load wheatprotein.txt
X=wheatprotein(:, 1 : 6);
Y=wheatprotein(:, 7);
u = bic_xenv(X, Y);
ModelOutput=xenv(X, Y, u);
TestOutout = testcoefficient_xenv(ModelOutput);
```

Test Hypothesis	Chisq Statistic	DF	P-value	
L * beta * R = A	3233.053	6	0.0000	

```
r = size(Y, 2);
p = size(X, 2);
TestInput.L = rand(2, p);
TestInput.R = rand(r, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_xenv(ModelOutput, TestInput);
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	33.578	2	0.0000

128 CHAPTER 8. XENV

### 8.9 xenv

Fit the envelope model for the reduction on X.

#### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

### **Syntax**

```
ModelOutput = xenv(X, Y, u)
ModelOutput = xenv(X, Y, u, Opts)
```

# Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

**u**: Dimension of the envelope. An integer between 0 and p.

**Opts**: A list containing the optional input parameter, to control the iterations in sg\_min. If one or several (even all) fields are not defined, the default settings are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the envelope subspace. An p by u matrix. Default value is the one generated by function get\_init.

### Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients  $\beta$ . An p by r matrix.
- ModelOutput.SigX: The envelope estimator of the covariance matrix of X,  $\Sigma_X$ . A p by p matrix
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. An p by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An p by p-u semi-orthogonal matrix.
- ModelOutput.eta: The coordinates of  $\beta$  with respect to Gamma. An u by r matrix.

8.9. XENV 129

• ModelOutput.Omega: The coordinates of  $\Sigma_X$  with respect to Gamma. An u by u matrix.

- ModelOutput.Omega0: The coordinates of  $\Sigma_X$  with respect to Gamma0. An p u by p u matrix.
- ModelOutput.mu: The estimated intercept. An r by 1 vector.
- ModelOutput.sigYcX: The estimated conditional covariance matrix of Y given X. An r by r matrix.
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of  $vec(\beta)$ . An pr by pr matrix. The covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1 / n.
- ModelOutput.asyXenv: 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 / sqrt(n).
- ModelOutput.ratio: The asymptotic standard error ratio of the standard multivariate linear regression estimator over the envelope estimator, for each element in  $\beta$ . An p by rmatrix
- ModelOutput.np: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

### **Description**

This function fits the envelope model in the predictor's space, using the maximum likelihood estimation. When the dimension of the envelope is between 1 and r - 1, we implemented the algorithm in Cook et al. (2012). 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

- 1. The codes are implemented based on the algorithm in Section 4.5.1 of Cook et al (2012).
- 2. The Grassmann manifold optimization step calls the package sg\_min 2.4.1 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

```
load wheatprotein.txt
X = wheatprotein(:, 1 : 6);
Y = wheatprotein(:, 7);

p = size(X, 2);
ModelOutput = xenv(X, Y, p);

% When u = p, the envelope model reduces to the ordinary least squares
% regression

temp = fit_OLS(X, Y);
temp.SigmaOLS
ModelOutput.sigYcX
temp.betaOLS'
ModelOutput.beta
```

130 CHAPTER 8. XENV

```
ans =
   0.0321
ans =
    0.0321
ans =
   -0.0416
  -0.0490
   0.3368
   -0.1981
   0.0020
   -0.0480
ans =
   -0.0416
  -0.0490
   0.3368
   -0.1981
   0.0020
   -0.0480
       u = bic\_xenv(X, Y);
       ModelOutput = xenv(X, Y, u)
ModelOutput =
         beta: [6x1 double]
         SigX: [6x6 double]
        Gamma: [6x4 double]
       Gamma0: [6x2 double]
          eta: [4x1 double]
        Omega: [4x4 double]
       OmegaO: [2x2 double]
           mu: 24.8863
       sigYcX: 0.0321
            1: -6.7737e+05
    covMatrix: [6x6 double]
      asyXenv: [6x1 double]
        ratio: [6x1 double]
          np: 27
```

n: 50

8.9. XENV 131

```
\% To compare with the results obtained by Partial Least Squares, use the
      % plsregress command
       [XL, YL, XS, YS, BETA, PCTVAR, MSE, stats] = plsregress(X, Y, u);
       ModelOutput.beta
       BETA(2 : end, :)
ans =
   -0.0443
   -0.0481
   0.3377
   -0.1963
   0.0019
   -0.0487
ans =
   -0.0199
   0.1373
    0.1309
   -0.1827
   0.0056
   -0.0708
```

# xenvpls

# 9.1 bstrp\_xenvpls

Compute bootstrap standard error of the envelope model for the reduction on X using partial least squares algorithm.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
bootse = bstrp_xenvpls(X, Y, u, B)
bootse = bstrp_xenvpls(X, Y, u, B, Opts)
```

### **Input**

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

**u**: Dimension of the envelope subspace. A positive integer between 0 and p.

**B**: Number of bootstrap samples. A positive integer.

**Opts**: A list containing the optional input parameters. If one or several (even all) fields are not defined, the default settings are used.

• Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

### Output

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

# **Description**

This function computes the bootstrap standard errors for the regression coefficients in the envelope model by bootstrapping the residuals. The envelope model is applied for the reduction on X, using the partial least squares algorithm.

```
load wheatprotein.txt
       X = wheatprotein(:, 1 : 6);
       Y = wheatprotein(:, 7);
       m = 5;
       u = mfoldcv\_xenvpls(X, Y, m)
u =
     6
       B = 100;
       bootse = bstrp_xenvpls(X, Y, u, B, Opts)
bootse =
    0.0287
    0.0383
    0.0409
    0.0207
    0.0026
    0.0097
```

134 CHAPTER 9. XENVPLS

# 9.2 mfoldcv\_xenvpls

Select the dimension of the envelope subspace using m-fold cross validation for envelope model on the reduction on X using partial least squares algorithm.

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
u = mfoldcv_xenvpls(X, Y, m)
u = mfoldcv_xenvpls(X, Y, m, Opts)
```

### Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

m: A positive integer that is used to indicate m-fold cross validation.

**Opts**: A list containing the optional input parameters. If one or several (even all) fields are not defined, the default settings are used.

• Opts.verbose: Flag for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

### Output

**u**: The dimension of the envelope subspace selected by m-fold cross validation.

### **Description**

This function implements m-fold cross validation to select the dimension of the envelope space, based on prediction performance. For each u, the data is partitioned into m parts, each part is in turn used for testing for the prediction performance while the rest m-1 parts are used for training. The dimension is select as the one that minimizes the average prediction errors. If Y is multivariate, the identity inner product is used for computing the prediction errors.

```
load wheatprotein.txt
X = wheatprotein(:, 1 : 6);
Y = wheatprotein(:, 7);
```

m = 5; u = mfoldcv\_xenvpls(X, Y, m)

u =

6

# 9.3 xenvpls

Fit the envelope model for the reduction on X using partial least squares algorithm.

### **Contents**

- Syntax
- Input
- Output
- Description
- Reference
- Example

### **Syntax**

```
ModelOutput = xenvpls(X, Y, u)
```

### Input

**X**: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The number of predictors should be greater than the number of the responses. And they must be continuous variables.

**Y**: Responses. An n by r matrix, r is the number of responses. The response can be univariate or multivariate and must be continuous variable.

**u**: Dimension of the envelope. An integer between 0 and p.

### Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients  $\beta$ . An p by r matrix.
- ModelOutput.SigX: The envelope estimator of the covariance matrix of X,  $\Sigma_X$ . A p by p matrix.
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. An p by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An p by p-u semi-orthogonal matrix.
- ModelOutput.eta: The coordinates of  $\beta$  with respect to Gamma. An u by r matrix.
- ModelOutput.Omega: The coordinates of  $\Sigma_X$  with respect to Gamma. An u by u matrix.
- ModelOutput.Omega0: The coordinates of  $\Sigma_X$  with respect to Gamma0. An p u by p u matrix.
- ModelOutput.mu: The estimated intercept. An r by 1 vector.
- ModelOutput.sigYcX: The estimated conditional covariance matrix of Y given X. An r by r matrix.
- ModelOutput.np: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

9.3. XENVPLS 137

### **Description**

This function fits the envelope model in the predictor's space, by the partial least squares algorithm in Cook et al. (2012). In the population level, this algorithm is equivalent to that in xenv.m, which uses the maximum likelihood estimation. In the sample version, the two algorithms are different. And this algorithm is much faster, which provides a root n consistent starting value for the one in xenv.m.

### Reference

The codes are implemented based on the algorithm in Section 4.3 of Cook et al (2012).

```
load wheatprotein.txt
       X = wheatprotein(:, 1 : 6);
       Y = wheatprotein(:, 7);
       m = 5;
       u = mfoldcv\_xenvpls(X, Y, m)
u =
     6
       ModelOutput = xenvpls(X, Y, u)
ModelOutput =
      beta: [6x1 double]
      SigX: [6x6 double]
     Gamma: [6x6 double]
    Gamma0: []
       eta: [6x1 double]
     Omega: [6x6 double]
    OmegaO: []
        mu: 24.5781
    sigYcX: 0.0321
        np: 29
         n: 50
       ModelOutput.beta
```

```
ans =
-0.0416
-0.0490
0.3368
-0.1981
```

138 CHAPTER 9. XENVPLS

0.0020

-0.0480

# auxiliary

# 10.1 center

Subtract the mean of each column.

### **Contents**

- Syntax
- Input
- Output
- Description

# **Syntax**

XC = center(X)

# Input

**X**: A matrix or a column vector.

# Output

**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 subtracting each column by its column mean.

### **10.2** Contr

Compute the contraction matrix of dimension r.

### **Contents**

- Syntax
- Input
- Output
- Description

### **Syntax**

```
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  $\operatorname{r}(r+1)/2$  vector. For more details of "vec", "vech", contraction and expansion matrix, refer to Henderson and Searle (1979).

10.3. EXPAN 141

# 10.3 Expan

Compute the expansion matrix of dimension r.

### **Contents**

- Syntax
- Input
- Output
- Description

### **Syntax**

```
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, vech(A) = Contr(r) \* vec(A), and vec(A) = Expan(r) \* 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).

# 10.4 fit\_OLS

Multivariate linear regression.

### **Contents**

- Syntax
- Input
- Output
- Description
- Example

### **Syntax**

```
ModelOutput = 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

**ModelOutput**: A list that contains the maximum likelihood estimators of regression coefficients and error covariance matrix.

- ModelOutput.betaOLS: An r by p matrix containing estimate of the regression coefficients  $\beta$ .
- ModelOutput.SigmaOLS: An r by r matrix containing estimate of the error covariance matrix.
- ModelOutput.alpha: An r by 1 vector containing estimate of the intercept.
- ModelOutput.n: The number of observations in the data. A positive integer.

### **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  $\varepsilon$ .

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1 : 6);
ModelOutput = fit_OLS(X, Y)
ModelOutput.betaOLS
ModelOutput.SigmaOLS
```

10.4. FIT\_OLS 143

# ModelOutput =

betaOLS: [6x1 double]
SigmaOLS: [6x6 double]
alpha: [6x1 double]

n: 50

ans =

3.2724

8.0288

7.5224

-2.0609

3.2244

0.6538

ans =

1.0e+03 \*

1.1905	0.9759	1.0506	1.1524	1.5384	0.6335
0.9759	0.8061	0.8657	0.9432	1.2636	0.5266
1.0506	0.8657	0.9310	1.0164	1.3664	0.5640
1.1524	0.9432	1.0164	1.1228	1.5234	0.6183
1.5384	1.2636	1.3664	1.5234	2.3229	0.8360
0.6335	0.5266	0.5640	0.6183	0.8360	0.3618

# 10.5 get\_envelope

Construct the envelope subspace using a sequential algorithm.

### **Contents**

- Syntax
- Input
- Output
- Description
- Reference

### **Syntax**

```
W = get_envelope(S, M, u)
```

### Input

**S**: An r by p matrix whose columns span the subspace, the rank of S cannot be greater than u.

**M**: An r by r positive semi-definite matrix.

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

### Output

**W**: An r by u semi-orthogonal matrix that spans the M-envelope of span(S).

# **Description**

This function constructs the M-envelope of span(S) using a sequential algorithm similar to partial least squares.

### Reference

The codes are implemented based on the algorithm in the lecture notes of Cook (2012).

```
S = [1 2 3]';
S0 = grams(nulbasis(S'));
M = S * S' + S0 * S0';
u = 1;
W = get_envelope(S, M, u)

W =

0.2673
0.5345
0.8018
```

10.6. GET\_INIT 145

# 10.6 get\_Init

Starting value for the envelope subspace.

### **Contents**

- Syntax
- Input
- Output
- Description
- Reference

### **Syntax**

```
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 are implemented based on the algorithm in Section 3.5 of Su and Cook (2011).

# 10.7 get\_Init4henv

Starting value for the heteroscedastic envelope subspace.

### **Contents**

- Syntax
- Input
- Output
- Description
- Reference

### **Syntax**

```
WInit = get_Init4henv(F, X, Y, u, DataParameter)
```

### Input

**F**: Objective function to get the heteroscedastic envelope subspace.

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

**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 heteroscedastic envelope subspace. An r by u orthogonal matrix.

### **Description**

We compute the eigenvectors for the estimated errors, and get r vectors. Then we get all the combinations of u vectors out of the r vectors. If the number of r 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 3 rounds and use the final set as our starting value.

### Reference

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

10.8. KPD

# 10.8 Kpd

Compute the communication matrix Kpd.

### **Contents**

- Syntax
- Input
- Output
- Description
- Reference

# **Syntax**

$$k = Kpd(p, d)$$

# Input

**p**, **d**: 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 are implemented based on Definition 3.1 in Magnus and Neudecker (1979).

# 10.9 Lmatrix

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

### **Contents**

- Syntax
- Input
- Output
- Description

# **Syntax**

```
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 Lmatrix(r) \* vec(A) will give the 2nd to the rth diagonal elements of A, arranged in a column vector.

10.10. MAKE\_DF

# 10.10 make\_dF

Generic function to generate the derivative function of the objective function F.

### **Contents**

- Syntax
- Input
- Output
- Description

### **Syntax**

dF = make\_dF(dfun\_method\_handle, FParameters)

### **Input**

- dfun\_method\_handle: A specific model derivative function of the objective function.
- FParameters: A structure that contains data parameters as input for the function dfun\_method\_handle.

### Output

• dF: The generic derivative function of the objective function for computing the envelope subspace.

# **Description**

Generic function to generate the derivative function of the objective function F. The function first sets a handle to the specific model function and fixes the data parameters from the sample needed for its computation. The handle fixed with those parameters is then evaluated at a given value for argument W. A generic derivative function dF is returned.

# 10.11 make\_F

Generic function to generate the objective function F.

### **Contents**

- Syntax
- Input
- Output
- Description

### **Syntax**

F = make\_F(fun\_method\_handle, FParameters)

# Input

- fun\_method\_handle: A specific model objective function.
- FParameters: A structure that contains data parameters as input for the function fun\_method\_handle.

### Output

• F: The generic objective function for computing the envelope subspace.

# **Description**

Generic function to generate the objective function F. The function first sets a handle to the specific model function and fixes the data parameters from the sample needed for its computation. The handle fixed with those parameters is then evaluated at a given value for argument W. A generic objective function F is returned.

# 10.12 make\_opts

Make optional input parameters for running the sg\_min package.

### **Contents**

- Syntax
- Input
- Output:
- Description

### **Syntax**

```
Opts = make_opts(Opts)
```

### Input

**Opts**: A list containing optional input parameter for sg\_min.m specified by users. One or several (even all) fields could be empty.

- Opts.maxIter: Maximum number of iterations.
- Opts.ftol: Tolerance parameter for F.
- Opts.gradtol: Tolerance parameter for dF.
- Opts.verbose: Flag for print out output, logical 0 or 1.

### **Output:**

**Opts**: A list containing optional input parameter for sg\_min.m, specified by users or the default values are used.

- Opts.maxIter: Maximum number of iterations. Default value: 300.
- Opts.ftol: Tolerance parameter for F. Default value: 1e-10.
- Opts.gradtol: Tolerance parameter for dF. Default value: 1e-7.
- Opts.verbose: Flag for print out output, logical 0 or 1. Default value: 0.

### **Description**

The sg\_min function has some optional input parameters that control the iteration process. These parameters include maximum number of iteration, tolerance parameters for convergence of the objective function F and the derivative of the objective function dF, and the print out of the iteration process. The user can set one or all of parameters, if not, default values will be used.

# 10.13 make\_parameter

Compute summary statistics from the data.

#### **Contents**

- Syntax
- Input
- Output
- Description

### **Syntax**

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', 'senv' or 'xenv'.

### Output

**DataParameter**: 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.

### 10.14 mtest

Perform Box's M test to check the homogeneity of the covariance matrices.

### **Contents**

- Syntax
- Input
- Output
- Description
- References
- Example

### **Syntax**

```
TestOutput = mtest(X, Y, alpha)
```

### Input

**X**: Group indicators. A matrix with n rows. X can only have p unique rows, where p is the number of groups. For example, if there are two groups, X can only have 2 different kinds of rows, such as (0, 1) and (1, 0), or (1, 0, 10) and (0, 5, 6). The number of columns is not restricted, as long as X only has p unique rows.

**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 greater than p.

alpha: Significance level for testing. A real number between 0 and 1, often taken at 0.05 or 0.01.

### Output

**TestOutput**: A list containing the Box's M statistic, the approximation test statistic, degrees of freedom for the approximation statistic test, and the p-value. At the same time, a table is printed out.

- TestOutput.mStatistic: The Box's M statistic. A real number.
- TestOutput.approxStatistic: The approximation test statistic.
- TestOutput.df: The degrees of freedom of the approximation statistic test. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].

# **Description**

This function performs the Box's M test for homegeneity of the covariance matrices for different groups, indicated by X. If the groups sample-size is at least 20 (sufficiently large), Box's M test takes a Chi-square approximation; otherwise it takes an F approximation.

10.14. MTEST 155

### References

The codes are implemented based on

Trujillo-Ortiz, A., R. Hernandez-Walls, K. Castro-Morales, A. Espinoza-Tenorio, A. Guia-Ramirez and R. Carmona-Pina. (2002). MBoxtest: Multivariate Statistical Testing for the Homogeneity of Covariance Matrices by the Box's M. A MATLAB file. [WWW document]. URL: http://www.mathworks.com/matlabcentral/fileexchange /loadFile.do?objectId=2733&objectType=FILE

# **Example**

```
load waterstrider.mat
alpha = 0.01;
TestOutput = mtest(X, Y, alpha);
```

MBox	Chi-sqr.	df	P		
157.5977	137.3361	72	0.0000		

Covariance matrices are significantly different.