# Matlab Toolbox Envelope: Reference Manual

# May 17, 2012

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# 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', '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.

 ${f u}$ : 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', '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 the number of bootstrap samples, logical 0 or 1. Default value: 0.

## Output

bootse: For 'env', 'henv', 'ienv', 'senv' and 'xenv', 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.

## **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 = \text{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
     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)
```

1.1. BOOTSTRAPSE 5

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 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
```

#### 1.4 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
```

## 1.5 modelselectlrt

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

#### **Contents**

- Svntax
- 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.

 ${f alpha}$ : 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: 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 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 = \text{wheatprotein}(:, 8);
     Y = \text{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
```

# 1.6 prediction

Perform estimation or prediction for models in the envelope family.

#### **Contents**

- Svntax
- 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 'peny'): 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.

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```
load wheatprotein.txt
     X = \text{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]
```

# SE: [4x1 double]

ans =

1.4680

0.4234

0.7145

0.3161

## 1.7 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, and the p-value. 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].

#### **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  $(L\beta R - A)$   $\hat{\Sigma}^{-1}$  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).

# **Example**

```
load wheatprotein.txt
    X = \text{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
```

0.0018

2

L \* beta \* R = A 12.598

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.

```
\begin{aligned} & load\ wheatprotein.txt \\ & X = wheatprotein(:,\,8); \\ & Y = wheatprotein(:,\,1:6); \\ & u = aic\_env(X,\,Y) \end{aligned}
```

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# 2.2 bic\_env

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

#### **Syntax**

```
\begin{array}{l} u = bic\_env(X, Y) \\ u = bic\_env(X, Y, Opts) \end{array}
```

#### 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 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)
```

u =

1

2.3. BSTRP\_ENV 23

# 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;
```

```
\begin{split} u &= lrt\_env(X,\,Y,\,alpha) \\ u &= \\ 1 \\ B &= 100; \\ bootse &= bstrp\_env(X,\,Y,\,u,\,B) \end{split}
```

bootse =

0.2893

0.4260

0.3523

0.5628

0.1675

0.6192

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# 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

Fit the envelope model.

#### **Contents**

- Svntax
- 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.

#### 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.

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 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 is 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).

# ${\bf ModelOutput} =$

beta: [6x1 double]
Sigma: [6x6 double]
Gamma: [6x1 double]
Gamma0: [6x5 double]
eta: 8.5647
Omega: 7.8762
Omega0: [5x5 double]
alpha: [6x1 double]
l: -850.7592
covMatrix: [6x6 double]
asyEnv: [6x1 double]
ratio: [6x1 double]
np: 28
n: 50

# ${\bf Model Output. Omega}$

ans =

7.8762

# eig(ModelOutput.Omega0)

ans =

1.0e+03\*

6.5166

0.2083

0.0201

0.0004

0.0003

# ModelOutput.ratio

ans =

28.0945

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18.4326

23.6384

16.3211

65.8245

6.4668

# 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.

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# 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.

 ${f alpha}$ : 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  $\alpha$ .

```
 \begin{aligned} & \text{load wheatprotein.txt} \\ & X = \text{wheatprotein}(:, \, 8); \\ & Y = \text{wheatprotein}(:, \, 1:6); \\ & \text{alpha} = 0.01; \\ & u = \text{lrt\_env}(X, \, Y, \, \text{alpha}) \end{aligned}
```

u =

1

2.8. PREDICT\_ENV 33

# 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.

```
\label{eq:continuous_section} \begin{split} & 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, :)'; \end{split}
```

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

```
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
```

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, and the p-value. 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].

# **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.

```
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
```

# henv

# 3.1 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

 $\boldsymbol{u}\!:$  Dimension of the envelope. An integer between 0 and r.

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# Description

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

# Example

```
\begin{aligned} & load\ waterstrider.mat \\ & u = aic\_henv(X,\,Y) \end{aligned}
```

6

u =

# 3.2 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)
```

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u =

4

# 3.3 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.

- 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 heteroscedastic envelope model by bootstrapping the residuals.

# Example

```
load waterstrider.mat
```

$$u = lrt\_henv(X,\,Y,\,0.01)$$

u =

6

$$\begin{split} B &= 100; \\ bootse &= bstrp\_henv(X, \, Y, \, u, \, B) \end{split}$$

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
0.0321	0.0463	0.0665

# 3.4 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.

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# 3.5 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.

#### 3.6 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.

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

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• 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 is 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]
     Omega0: [2x2 double]
       np: 98
        l: 1.0051e+03
   covMatrix: [32x32 double]
    asyHenv: [8x3 double]
     ratio: [8x3 double]
        ng: [3x1 double]
ans =
   6.5439 \quad 11.2830
                     6.4954
  4.6325 \quad 5.3226
                    4.7242
  4.4456 \quad 5.0741
                    4.4198
  4.7338
          6.2469
                    5.1937
  8.0377 12.5386
                    9.4823
  9.5067 11.5974 11.3444
  11.8632 15.6080 12.5611
  6.9792 11.1559 10.1002
```

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# 3.7 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

6

```
\begin{aligned} & load\ waterstrider.mat \\ & u = lrt\_henv(X,\,Y,\,0.01) \end{aligned} u =
```

# 3.8 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.

```
\begin{split} & \text{load waterstrider.mat} \\ & u = \text{lrt\_henv}(X,\,Y,\,0.01); \\ & \text{ModelOutput} = \text{henv}(X,\,Y,\,u); \\ & \text{ModelOutput.groupInd} \\ & \text{ModelOutput.mug} \\ & \text{Xnew} = X(1,\,:)' \end{split}
```

```
ans =
  -1
       -1
   0
        1
   1
        0
ans =
  -1.1417 -1.1267 -1.0845
  -1.4063 -1.4067 -1.3132
  -1.3314 -1.3336 -1.2152
  -0.3113 -0.1839 -0.1736
  0.4003 \quad 0.3847 \quad 0.3072
  0.4107 \quad 0.3753 \quad 0.3735
          0.3271 \quad 0.3179
  0.3467
  -0.1954 -0.2100 -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')
     {\bf 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
```

# 3.9 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, and the p-value. 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].

## **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
                                        0.0000
                               16
    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

# 4.1 aic\_ienv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
\begin{array}{l} u = aic\_ienv(X, Y) \\ u = aic\_ienv(X, Y, Opts) \end{array}
```

#### 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

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

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# Description

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

```
\begin{aligned} & load \ irisf.mat \\ & u = aic\_ienv(X, \, Y) \end{aligned} u =
```

# 4.2 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.

```
\begin{aligned} & load\ irisf.mat \\ u &= bic\_ienv(X,\,Y) \end{aligned} u =
```

4.3. BSTRP\_IENV 59

# 4.3 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.

```
u = bic ienv(X, Y)
```

```
\label{eq:B} \begin{split} \mathbf{u} &= \\ \mathbf{1} \\ \mathbf{B} &= 100; \\ \mathbf{bootse} &= \mathbf{bstrp\_ienv}(\mathbf{X},\,\mathbf{Y},\,\mathbf{u},\,\mathbf{B}) \end{split}
```

bootse =

13.4695 4.9601 7.4709 2.7315 14.9316 5.2913 8.7597 3.0853 4.4. DF4IENV 61

# 4.4 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.

# 4.5 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.

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#### **4.6** 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.

#### 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.
- 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 β.

- 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 is 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**

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

```
\begin{aligned} \text{load irisf.mat} \\ d &= \text{bic\_ienv}(X,\,Y) \\ d &= \end{aligned}
```

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# $\begin{aligned} & ModelOutput = ienv(X, \, Y, \, d) \\ & 1 - 1 \, . / \, ModelOutput.ratio \end{aligned}$

# ${\bf ModelOutput} =$

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 l: -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

# 4.7 lrt\_ienv

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

#### **Contents**

- Syntax
- Input
- Output
- Description
- Example

## **Syntax**

```
\begin{split} u &= lrt\_ienv(X, \, Y, \, alpha) \\ u &= lrt\_ienv(X, \, Y, \, alpha, \, Opts) \end{split}
```

#### 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  $\alpha$ .

```
\begin{aligned} & load \ irisf.mat \\ & alpha = 0.01; \\ & u = lrt\_ienv(X, Y, alpha) \end{aligned}
```

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u =

1

# 4.8 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.

```
\label{eq:continuity} \begin{split} & 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 \end{split}
```

```
PredictOutput = \\
      value: [4x1 double]
   covMatrix: [4x4 double]
        SE: [4x1 double]
ans =
  49.9458 \quad 51.0000
  34.2592 35.0000
  14.5771 14.0000
  2.4513 \quad 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
   2.0642
```

# 4.9 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, and the p-value. 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].

#### **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

# 5.1 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

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

5.1. AIC\_PENV 73

# Description

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

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# 5.2 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

**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.

5.2. BIC\_PENV 75

```
\begin{aligned} & \text{load fiberpaper.dat} \\ & Y = \text{fiberpaper}(:, 1:4); \\ & X temp = \text{fiberpaper}(:, 5:7); \\ & X.X1 = X temp(:, 3); \\ & X.X2 = X temp(:, 1:2); \\ & u = \text{bic\_penv}(X, Y) \end{aligned}
```

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# 5.3 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
```

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# 5.4 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.

 ${\it alpha}$ : 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  $\alpha$ .

5.4. LRT\_PENV 79

# Example

1

```
\label{eq:continuous_problem} \begin{split} & \text{load fiberpaper.dat} \\ & Y = \text{fiberpaper}(:,\,1:4); \\ & \text{Xtemp} = \text{fiberpaper}(:,\,5:7); \\ & \text{X.X1} = \text{Xtemp}(:,\,3); \\ & \text{X.X2} = \text{Xtemp}(:,\,1:2); \\ & \text{alpha} = 0.01; \\ & \text{u} = \text{lrt\_penv}(\text{X},\,\text{Y},\,\text{alpha}) \end{split}
```

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# 5.5 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.

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

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• 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.
- ModelOutput.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 is 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).

```
\label{eq:continuous_section} \begin{split} & \text{load fiberpaper.dat} \\ & Y = \text{fiberpaper}(:, 1:4); \\ & \text{Xtemp} = \text{fiberpaper}(:, 5:7); \\ & \text{X.X1} = \text{Xtemp}(:, 3); \\ & \text{X.X2} = \text{Xtemp}(:, 1:2); \\ & \text{alpha} = 0.01; \\ & \text{u} = \text{lrt\_penv}(X, Y, \text{alpha}) \end{split}
```

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```
u =
   1
     ModelOutput = penv(X, Y, u)
     {\bf Model Output. Omega}
     eig(ModelOutput.Omega0)
     ModelOutput.ratio
{\bf 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

# 5.6 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.

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```
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);
     X_{\text{new.}}X_{1} = X_{\cdot}X_{1}(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 \quad 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

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# 5.7 testcoefficient\_penv

This function tests the null hypothesis L \* beta \* R = A versus the alternative hypothesis L \* beta \* R  $\stackrel{\sim}{}$  = 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  $\beta$  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 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, and the p-value. 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].

#### **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 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  $\beta = 0$ . 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 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

## 6.1 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.

6.1. AIC\_SENV 89

```
\begin{aligned} & load('sales.txt') \\ & Y = sales(:,\,4:7); \\ & X = sales(:,\,1:3); \\ & u = aic\_senv(X,\,Y) \end{aligned}
```

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## 6.2 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

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

#### **Description**

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

```
\begin{aligned} & load('sales.txt') \\ & Y = sales(:, 4:7); \\ & X = sales(:, 1:3); \\ & u = bic \ senv(X, Y) \end{aligned}
```

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u =

2

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# 6.3 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);
```

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

u =

2

$$\begin{split} B &= 20; \\ bootse &= bstrp\_senv(X, \, Y, \, u, \, B) \end{split}$$

bootse =

0.0539	0.0472	0.0554
0.0675	0.0912	0.1178
0.0567	0.0781	0.0791
0.0986	0.0944	0.1283

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## 6.4 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.

6.5. F4SENV 95

## 6.5 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.

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# 6.6 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.

# 6.7 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.

```
\begin{split} & \operatorname{load}(\operatorname{'sales.txt'}) \\ & Y = \operatorname{sales}(:,\,4:7); \\ & X = \operatorname{sales}(:,\,1:3); \\ & u = \operatorname{bic\_senv}(X,\,Y); \\ & \operatorname{ModelOutput} = \operatorname{senv}(X,\,Y,\,u); \\ & \operatorname{Xnew} = X(1,\,:)'; \\ & \operatorname{PredictOutput} = \operatorname{predict\_senv}(\operatorname{ModelOutput},\,\operatorname{Xnew},\,\operatorname{'estimation'}) \end{split}
```

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# [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
```

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#### 6.8 senv

Fit the scaled envelope model.

#### **Contents**

- Syntax
- 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.

#### 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.
- ModelOutput.eta: The coordinates of  $\beta$  with respect to Gamma. An u by p matrix.

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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  $vec(\beta)$ . 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 is 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).

```
\begin{aligned} & load('sales.txt') \\ & Y = sales(:,\,4:7); \\ & X = sales(:,\,1:3); \\ & u = bic\_senv(X,\,Y) \end{aligned} u = \\ & 2 \\ & ModelOutput = senv(X,\,Y,\,u) \\ & ModelOutput.Lambda \\ & 1 - 1 \; . / \; ModelOutput.ratio \end{aligned}
```

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## ${\bf ModelOutput} =$

beta: [4x3 double]
Sigma: [4x4 double]
Lambda: [4x4 double]
Gamma: [4x2 double]
Gamma0: [4x2 double]
eta: [2x3 double]
Omega: [2x2 double]
Omega0: [2x2 double]
alpha: [4x1 double]
np: 23
l: -386.1900
covMatrix: [12x12 double]
asySenv: [4x3 double]
ratio: [4x3 double]
n: 50

ans =

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

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

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## 6.9 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, and the p-value. 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].

#### **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.

## **Example**

```
\begin{split} & \operatorname{load}(\operatorname{'sales.txt'}) \\ & Y = \operatorname{sales}(:,4:7); \\ & X = \operatorname{sales}(:,1:3); \\ & u = \operatorname{bic\_senv}(X,Y) \\ & \operatorname{ModelOutput} = \operatorname{senv}(X,Y,u); \\ & \operatorname{TestOutout} = \operatorname{testcoefficient\_senv}(\operatorname{ModelOutput}); \end{split}
```

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

\_\_\_\_\_

```
\begin{split} 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); \end{split}
```

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

## xenv

## 7.1 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**

```
\begin{array}{l} u = aic\_xenv(X, Y) \\ u = aic\_xenv(X, Y, Opts) \end{array}
```

## 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 p.

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# Description

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

```
\begin{aligned} & \text{load wheatprotein.txt} \\ & X = \text{wheatprotein}(:, 1:6); \\ & Y = \text{wheatprotein}(:, 7); \\ & u = \text{aic\_xenv}(X, Y) \end{aligned} u = \underbrace{4}
```

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## 7.2 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. 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:

#### 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.

```
 \begin{aligned} & \text{load wheatprotein.txt} \\ & X = \text{wheatprotein(:, 1 : 6);} \\ & Y = \text{wheatprotein(:, 7);} \\ & u = \text{bic } xenv(X, Y) \end{aligned}
```

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u =

4

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## 7.3 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. 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 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);
```

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```
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
```

 $\begin{array}{c} 0.0413 \\ 0.0167 \\ 0.0022 \\ 0.0087 \end{array}$ 

# 7.4 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.

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### 7.5 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.

# 7.6 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. 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.

 ${f alpha}$ : 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  $\alpha$ .

### **Example**

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

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$$\begin{aligned} & alpha = 0.01; \\ & u = lrt\_xenv(X,\,Y,\,alpha) \end{aligned}$$

u =

4

# 7.7 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.

### **Example**

```
\label{eq:continuous_section} \begin{split} & 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') \end{split}
```

[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')
     {\bf PredictOutput.SE}
PredictOutput =
     value: 9.1751
  covMatrix: 16.8760
       SE: 4.1080
ans =
  4.1080
```

# 7.8 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  $I_n$ .
- 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, and the p-value. 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].

### **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.

# **Example**

```
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
```

### **7.9** 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. 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 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.

### 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.

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• 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(β). 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 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.

### **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. (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 r and r are uncorrelated, and the fitting is different.

### References

- 1. The codes is 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).

### **Example**

```
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
```

```
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]
     Omega0: [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 7.9. XENV 121

```
\% 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

# auxiliary

# 8.1 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.

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### 8.2 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).

# 8.3 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).

8.4. FIT\_OLS 125

# 8.4 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  $\varepsilon$ .

### **Example**

```
load wheatprotein.txt

X = wheatprotein(:, 8);

Y = wheatprotein(:, 1 : 6);

ModelOutput = fit_OLS(X, Y)

ModelOutput.betaOLS

ModelOutput.SigmaOLS
```

# ${\bf ModelOutput} =$

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

8.5. GET\_INIT 127

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

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

8.7. KPD 129

# 8.7 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 is implemented based on Definition 3.1 in Magnus and Neudecker (1979).

# 8.8 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.

8.9. MAKE\_DF

# 8.9 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.

# 8.10 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.

8.11. MAKE\_OPTS 133

# 8.11 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.

# 8.12 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.

# 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.