MATLAB Toolbox envlp: Reference Manual

June 10, 2014

Introduction

The toolbox "envlp" provides MATLAB functions that fit a variety of envelope models for multivariate analysis, especially multivariate linear regression. This document contains the complete description of this toolbox. It includes information on syntax and semantics, description and example for the functions in the toolbox. This manual is intended for users who need detailed information on the structure of the toolbox and its functions. It is also helpful to advanced users who want to write extensions for the toolbox.

The content of each module is as follows:

tools Functions for dimension selection and inference.

env Functions that implement the envelope model.

envseq Functions that implement the envelope model using sequential algorithm.

henv Functions that implement the heteroscedastic envelope model.

ienv Functions that implement the inner envelope model.

penv Functions that implement the partial envelope model.

senv Functions that implement the scaled envelope model.

xenv Functions that implement the envelope model in the predictor space.

xenvpls Functions that implement the envelope model in the predictor space using partial least squares algorithm.

envmean Functions that implement the envelope estimator of the multivariate mean.

auxiliary Auxiliary functions used internally in the toolbox.

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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 methods 'env', 'envpls', 'henv', 'ienv', ' senv', 'xenv' and 'xenvpls'. X is an n by p matrix, p is the number of predictors.

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

- X.X1 (only for 'penv'): Predictors of main interest. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X.X2 (only for 'penv'): Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates.
- **Y**: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.
- ${\bf u}$: Dimension of the envelope subspace. The legitimate range of u depends on the model specified.
- **B**: Number of bootstrap samples. A positive integer.

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

Opts: A list containing the optional input parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: For 'env', 'envpls', 'henv', 'ienv', and 'senv', an r by p matrix containing the standard errors for elements in β computed by bootstrap. For 'penv', an r by p1 matrix containing the standard errors for β_1 computed by bootstrap. For 'xenv' and 'xenvpls', a p by r matrix containing the standard errors for elements in β 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 = modelselectlrt(X, Y, alpha, 'env');
     B = 100;
     modelType = 'env';
     bootse = bootstrapse(X, Y, u, B, modelType)
bootse =
   0.2896
   0.4352
   0.3189
   0.5735
   0.2543
   0.5840
     modelType = 'envpls';
     bootse = bootstrapse(X, Y, u, B, modelType)
```

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```
bootse =
  9.3899
   7.7384
   8.3303
  9.0875
  13.4416
  5.1477
     load fiberpaper.dat
     Y = fiberpaper(:, 1 : 4);
     X.X1 = fiberpaper(:, 7);
     X.X2 = fiberpaper(:, 5:6);
     alpha = 0.01;
     u = modelselectlrt(X, Y, alpha, 'penv');
     B = 100;
     modelType = 'penv';
     bootse = bootstrapse(X, Y, u, B, modelType)
```

bootse =

0.0027

0.0012

0.0020

0.0009

1.2 bootstrapse_OLS

Compute bootstrap standard error for ordinary least squares.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
bootse = bootstrapse OLS(X, Y, B)
```

Input

X: Predictors, an n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.

Y: Multivariate responses, an n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

B: Number of bootstrap samples. A positive integer.

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

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

Output

bootse: The standard error for elements in β 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 mfoldcy

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

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

- X.X1 (only for 'penv'): Predictors of main interest. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X.X2 (only for 'penv'): Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates.

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

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

modelType: A string of characters indicting the model, choices can be 'env', 'envseq', 'henv', 'ienv', 'penv', 'senv', 'xenv' or 'xenvpls'.

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

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Output

SelectOutput: A list containing the results of the selection.

• SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and r.

• SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

```
\label{eq:continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous_continuous
```

1.4 modelselectaic

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{split} u &= modelselectaic(X, \, Y, \, modelType) \\ u &= modelselectaic(X, \, Y, \, modelType, \, Opts) \end{split}
```

Input

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

For model type '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 of characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv', 'senv' and 'xenv'.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

13

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 =

load fiberpaper.dat
   Y = fiberpaper(:, 1 : 4);
   X.X1 = fiberpaper(:, 7);
   X.X2 = fiberpaper(:, 5 : 6);
   modelType = 'penv';
   u = modelselectaic(X, Y, modelType)

u =

3
```

1.5 modelselectbic

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

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

Input

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

For model type '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 of characters indicting the model, choices can be 'env', 'henv', 'ienv', 'penv', 'senv' and 'xenv'.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. 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 =

load fiberpaper.dat
   Y = fiberpaper(:, 1 : 4);
   X.X1 = fiberpaper(:, 7);
   X.X2 = fiberpaper(:, 5 : 6);
   modelType = 'penv';
   u = modelselectbic(X, Y, modelType)

u =

1
```

1.6 modelselectlrt

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

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

- X.X1 (only for 'penv'): Predictors of main interest. An n by p1 matrix, n is the number of observations, and p1 is the number of main predictors. The predictors can be univariate or multivariate, discrete or continuous.
- X.X2 (only for 'penv'): Covariates, or predictors not of main interest. An n by p2 matrix, p2 is the number of covariates.

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

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

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

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. 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 = wheatprotein(:, 8);
     Y = wheatprotein(:, 1:6);
     alpha = 0.01;
     modelType = 'env';
     u = modelselectlrt(X, Y, alpha, modelType)
u =
   1
     load fiberpaper.dat
     Y = fiberpaper(:, 1 : 4);
     X.X1 = fiberpaper(:, 7);
     X.X2 = fiberpaper(:, 5:6);
     alpha = 0.01;
     modelType = 'penv';
     u = modelselectlrt(X, Y, alpha, modelType)
u =
   1
```

1.7 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 of 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 = prediction(ModelOutput, Xnew, 'estimation', modelType)
     [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);
     X.X1 = fiberpaper(:, 7);
     X.X2 = fiberpaper(:, 5:6);
     modelType = 'penv';
     u = modelselectbic(X, Y, modelType);
     ModelOutput = penv(X, Y, u);
     X_{new.X1} = X_{.X1(1, :)};
     Xnew.X2 = X.X2(1, :)';
     PredictOutput = prediction(ModelOutput, Xnew, 'estimation', modelType)
     PredictOutput.SE
PredictOutput =
     value: [4x1 double]
   covMatrix: [4x4 double]
       SE: [4x1 double]
```

ans =

1.4680

0.4234

0.7145

0.3161

1.8 testcoefficient

This function tests the null hypothesis L^* beta *R = A versus the alternative hypothesis L^* beta *R = 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 of 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 β 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 β on the right. According to different model, it has different size requirement. Default value will be set if the user does not specify.
- TestInput.A: The matrix on the right hand side of the equation. Default value will be set if the user does not specify.

Output

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

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

Description

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

```
\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); \\ & ModelOutput = 'env'; \\ & TestOutout = testcoefficient(ModelOutput, modelType); \end{split}
```

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

```
\label{eq:load-fiberpaper.dat} \begin{split} &Y = \text{fiberpaper}(:, 1:4); \\ &X.X1 = \text{fiberpaper}(:, 7); \\ &X.X2 = \text{fiberpaper}(:, 5:6); \\ &\text{alpha} = 0.01; \\ &u = \text{modelselectlrt}(X, Y, \text{alpha, 'penv'}); \\ &\text{ModelOutput} = \text{penv}(X, Y, u); \\ &r = \text{size}(Y, 2); \\ &p1 = \text{size}(X.X1, 2); \\ &\text{TestInput.L} = \text{rand}(2, r); \\ &\text{TestInput.R} = \text{rand}(p1, 1); \\ &\text{TestInput.A} = \text{zeros}(2, 1); \\ &\text{TestOutout} = \text{testcoefficient} \quad \text{penv}(\text{ModelOutput, TestInput}); \end{split}
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	12.598	2	0.0018

env

2.1 aic_env

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = aic_{env}(X, Y)

u = aic_{env}(X, Y, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. 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}
```

2.2. BIC_ENV 25

2.2 bic env

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = bic_env(X, Y)

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.

Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. 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.

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

u =

1

2.3. BSTRP_ENV 27

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 parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in β 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\ wheat protein.txt
     X = wheatprotein(:, 8);
     Y = wheatprotein(:, 1:6);
     alpha = 0.01;
     u = modelselectlrt(X,\,Y,\,alpha,\,{}'env')
u =
  1
     B = 100;
     bootse = bstrp\_env(X, Y, u, B)
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

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

Syntax

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

Input

X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

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

Opts: A list containing the optional input parameters, 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 to print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the envelope subspace. An r by u matrix. Default value is the one generated by function get_Init.

Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients β . 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 β with respect to Gamma. A u by p matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. A 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.asySE: The asymptotic standard error for elements in β 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 β . An r by p matrix
- ModelOutput.paramNum: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

Description

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

References

- 1. The codes are implemented based on the algorithm in Section 4.3 of Cook et al (2010).
- 2. The Grassmann manifold optimization step calls the package sg_min 2.4.3 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]
asySE: [6x1 double]
ratio: [6x1 double]
paramNum: 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

${\bf Model Output. ratio}$

ans =

28.0389

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18.3983

23.5916

16.2928

65.7999

6.4555

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.

2.7. LRT_ENV 35

2.7 lrt env

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{split} u &= lrt\_env(X,\,Y,\,alpha) \\ u &= lrt\_env(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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. 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 α .

```
\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 = \underbrace{1}
```

2.8 mfoldcv env

Select the dimension of the envelope subspace using m-fold cross validation.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
SelectOutput = mfoldcv_env(X, Y, m)
SelectOutput = mfoldcv_env(X, Y, m, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations.

Y: Responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and r.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

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Description

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

Example

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1 : 6);
Opts.table = 1; % Print out the table of average prediction error for each u
SelectOutput = mfoldev env(X, Y, 5, Opts);
```

u	CV error
0	88.327
1	88.222
2	88.229
3	88.343
4	90.176
5	89.449
6	90.284

SelectOutput.u

```
ans =  1  Opts.perm = 10; % Run 5-fold CV on 10 permutations Opts.seed = 3; % Set seed for the permutations Opts.table = 1; SelectOutput = mfoldcv_env(X, Y, 5, Opts);
```

```
0 83.858
1 83.754
2 83.837
3 84.847
4 84.943
```

```
5 84.451
6 85.733
```

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

SelectOutput.PreErr

```
ans =
  83.8414
          83.7358
                  83.7703 84.4435 84.9735 84.3271
                                                     86.0893
  85.1301
          85.0230
                   85.0517
                            87.3159
                                    86.8758
                                             85.7392
                                                     87.3486
  82.8522
          82.7447
                   83.1461
                           85.1392
                                    84.6682
                                             84.2123
                                                     85.6514
                                    83.9716 85.0202 85.0807
  84.0505
          83.9447
                   83.9708
                           83.9715
  83.2022
          83.0987
                   83.1268
                           83.1323
                                    83.7480
                                             84.1540
                                                     84.1109
  83.4689
          83.3656
                   83.4763
                           87.8617
                                    87.8145
                                             84.4186
                                                     90.1180
                                    85.5000
  84.9664
          84.8683
                   84.9066
                           84.9103
                                             84.9104
                                                     85.5247
  85.2560
          85.1521
                   85.2284
                            85.2295
                                    86.0263
                                             86.0263
                                                      86.7444
  82.6187
          82.5142
                  82.5512
                            83.2121
                                    82.7440 82.5517
                                                      83.4039
  83.1972
          83.0933
                  83.1446
                           83.2518
                                    83.1093 83.1452
                                                      83.2577
```

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

```
ans = 83.8583 \quad 83.7541 \quad 83.8373 \quad 84.8468 \quad 84.9431 \quad 84.4505 \quad 85.7330
```

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans =  0.9663 \quad 0.9670 \quad 0.9323 \quad 1.6501 \quad 1.6368 \quad 1.0620 \quad 2.0453
```

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2.9 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} & \text{load wheatprotein:} xt \\ & X = \text{wheatprotein:} (:, 8); \\ & Y = \text{wheatprotein:} (:, 1:6); \\ & \text{alpha} = 0.01; \\ & u = \text{lrt\_env}(X, Y, \text{alpha}); \\ & \text{ModelOutput} = \text{env}(X, Y, u); \\ & X \text{new} = 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')
     {\bf 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
```

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ans =

34.9161

28.7280

30.8775

33.9006

48.6945

19.2448

2.10 predict2_env

Perform estimation or prediction under the envelope model through partial envelope model.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

PredictOutput = predict2 env(X, Y, Xnew, infType)

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.

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
- 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. Compared to predict_env, this function performs prediction through partial envelope model, which can be more accurate if the partial envelope is of smaller dimension and contains less variant material information.

References

1. The codes are implemented based on the following reference: R.D. Cook (2013) "Lecture Notes on Envelope Models and Methods." School of Statistics, University of Minnesota, Minneapolis.

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```
load fiberpaper.dat
     Y = fiberpaper(:, 1 : 4);
     X = fiberpaper(:, [7 5 6]);
     alpha = 0.01;
     u = lrt_{env}(X, Y, alpha);
     ModelOutput = env(X, Y, u);
     Xnew = X(10, :)';
     p1 = predict_env(ModelOutput, Xnew, 'estimation')
p1 =
      value: [4x1 double]
   covMatrix: [4x4 double]
        SE: [4x1 double]
     p1.value
ans =
  20.1120
   6.9174
   4.7911
   0.6162
     p1.SE
ans =
   1.7555
   0.4533
   0.8248
   0.3846
     p2 = predict2_env(X, Y, Xnew, 'estimation')
p2 =
      value: [4x1 double]
   covMatrix: [4x4 double]
        SE: [4x1 double]
     p2.value
```

ans =

20.1595

6.9105

4.8021

0.6182

p2.SE

ans =

0.2591

0.1001

0.1459

0.0741

p1.SE./p2.SE

ans =

6.7766

4.5264

5.6532

5.1914

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2.11 testcoefficient env

This function tests the null hypothesis L^* beta *R = A versus the alternative hypothesis L^* beta *R = 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 β 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 β on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix I_n .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

Output

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

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

Description

This function tests for hypothesis $H_0: L\beta R = A$, versus $H_\alpha: L\beta R \neq A$. The β 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.

```
\begin{split} & \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}); \\ & \text{ModelOutput} = \text{env}(X, Y, u); \\ & \text{TestOutout} = \text{testcoefficient\_env}(\text{ModelOutput}); \end{split}
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	116.230	6	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\_env(ModelOutput,\,TestInput); \end{split}
```

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	111.628	2	0.0000

envmean

3.1 aic_envmean

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = aic\_envmean(Y)

u = aic\_envmean(Y, Opts)
```

Input

Y: Data matrix. An n by p matrix, p is the dimension of the variable and n is number of observations.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

Description

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

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```
\begin{aligned} & load \ Adopted \\ & Y = Adopted(:, 1:6); \\ & u = aic\_envmean(Y) \end{aligned} u = 3
```

3.2 bic envmean

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = bic_envmean(Y)
u = bic_envmean(Y, Opts)
```

Input

Y: Data matrix. An n by p matrix, p is the dimension of the variable and n is number of observations.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

Description

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

```
\begin{aligned} & \text{load Adopted} \\ & Y = \text{Adopted}(:, 1:6); \\ & u = \text{bic\_envmean}(Y) \end{aligned} u = 3
```

3.3 bstrp_envmean

Compute bootstrap standard error for the envelope estimator of the multivariate mean.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
bootse = bstrp_envmean(Y, u, B)
bootse = bstrp_envmean(Y, u, B, Opts)
```

Input

Y: Data matrix. An n by p matrix, p is the dimension of the variable and n is number of observations.

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

Opts: A list containing the optional input parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in μ computed by bootstrap. A p dimensional column vector.

Description

This function computes the bootstrap standard errors for the envelope estimator of the multivariate mean by bootstrapping the residuals.

```
\begin{aligned} & load \ Adopted \\ & Y = Adopted(:, 1:6); \\ & u = bic\_envmean(Y) \end{aligned}
```

22.0329

```
u = 3
B = 100;
bootse = bstrp\_envmean(Y, u, B)
bootse = 0.5155
13.4169
13.2268
17.0221
21.4016
```

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3.4 dF4envmean

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

```
df = dF4envmean(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: A p by u matrix containing the value of the derivative function evaluated at R.

Description

The objective function is derived by maximum likelihood estimation. This function is the derivative of the objective function.

3.5 envmean

Provide envelope estimator for the multivariate mean.

Contents

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

Syntax

```
ModelOutput = envmean(Y, u)
ModelOutput = envmean(Y, u, Opts)
```

Input

Y: Data matrix. An n by p matrix, p is the dimension of the variable and n is number of observations.

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

Opts: A list containing the optional input parameters, 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 to print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the envelope subspace. A p by u matrix. Default value is the one generated by function get_Init4envmean.

Output

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

- ModelOutput.mu: The envelope estimator of the multivariate mean μ . A p dimensional column vector.
- ModelOutput.Sigma: The envelope estimator of the error covariance matrix. A p by p matrix.
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. A p by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. A p by p-u semi-orthogonal matrix.
- Model Output.eta: The coordinates of μ with respect to Gamma. A u dimensional column vector
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. A u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. A p-u by p-u matrix.

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- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of μ . A p by p matrix. The covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1/n.
- ModelOutput.asySE: The asymptotic standard error for elements in μ under the envelope model. A p dimensional column vector. 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 μ . A p dimensional column vector.
- ModelOutput.paramNum: 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 provides an envelope estimator for the multivariate mean, with a given dimension of the envelope subspace u. The estimator is obtained using the maximum likelihood estimation. When the dimension is p, then the envelope model degenerates to the standard sample mean. When the dimension is 0, it means that Y has mean 0.

References

The Grassmann manifold optimization step calls the package sg_min 2.4.3 by Ross Lippert (http://web.mit.edu/~ripper/www.sgmin.html).

Example

```
load Adopted
Y = Adopted(:, 1 : 6);
u = bic_envmean(Y)

u =

3

ModelOutput = envmean(Y, u)

ModelOutput =

mu: [6x1 double]
Sigma: [6x6 double]
Gamma: [6x3 double]
Gamma0: [6x3 double]
eta: [3x1 double]
Omega: [3x3 double]
Omega0: [3x3 double]
1: -1.3492e+03
```

covMatrix: [6x6 double]

asySE: [6x1 double] ratio: [6x1 double] paramNum: 24 n: 62

${\bf Model Output.mu}$

ans =

12.3258

85.9841

115.5767

112.1291

114.4862

106.4240

ModelOutput.Sigma

ans =

Columns 1 through 5

8.3278	2.9150	-4.0008	0.1057	0.3731
2.9150	235.6587	5.8146	42.1613	59.7492
-4.0008	5.8146	179.2066	91.7228	92.9563
0.1057	42.1613	91.7228	167.1073	114.4203
0.3731	59.7492	92.9563	114.4203	184.3248
-0.8157	71.9394	72.1815	110.2918	161.8752

Column 6

-0.8157

71.9394

72.1815

110.2918

161.8752

233.9185

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3.6 F4envmean

Objective function for computing the envelope subspace.

Contents

- Syntax
- Input
- Output
- Description

Syntax

```
f = F4envmean(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 by maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace.

3.7 lrt envmean

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = lrt_envmean(Y, alpha)

u = lrt_envmean(Y, alpha, Opts)
```

Input

Y: Data matrix. An n by p matrix, p is the dimension of the variable and n is number of observations.

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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. 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, with pre-specified significance level α .

```
load Adopted
Y = Adopted(:, 1 : 6);
alpha = 0.01;
u = lrt envmean(Y, alpha)
```

 $\mathbf{u} =$

2

3.8 mfoldcv envmean

Select the dimension of the envelope subspace using m-fold cross validation.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
SelectOutput = mfoldcv_envmean(Y, m)
SelectOutput = mfoldcv_envmean(Y, m, Opts)
```

Input

Y: Data matrix. An n by p matrix, p is the dimension of the variable and n is number of observations.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and r.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
\label{eq:continuous_section} \begin{split} & load\ Adopted\\ & Y = Adopted(:,1:6);\\ & Opts.table = 1;\ \%\ Print\ out\ the\ table\ of\ average\ prediction\ error\ for\ each\ u\\ & SelectOutput = mfoldcv\_envmean(Y,5,Opts); \end{split}
```

u	CV error
0	68.402
1	3.321
2	31.070
3	30.267
4	3.324
5	3.324
6	3.323

SelectOutput.u

```
ans =

1

Opts.perm = 10; % Run 5-fold CV on 10 permutations
Opts.seed = 3; % Set seed for the permutations
Opts.table = 1;
SelectOutput = mfoldcv_envmean(Y, 5, Opts);
```

u	CV error
0	68.381
1	23.071
2	11.282
3	5.411
4	2.838
5	2.838
6	2.839

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

 ${\bf SelectOutput.PreErr}$

ans =

68.4179 30.0985 31.6848 3.25553.2601 3.2623 3.2629 68.3949 3.0342 3.0239 3.0259 3.0180 3.0145 3.0191 2.6861 2.67492.6823 68.4065 2.6867 2.6826 2.6790 68.3404 2.45182.44962.4490 2.4441 2.4512 2.451768.3574 31.4960 3.9833 3.9791 3.9760 3.9775 3.9768 68.3996 30.1065 2.5022 2.5039 2.5026 2.50582.4999 68.3919 41.4619 2.0116 $2.0079 \quad 27.7202$ 2.0073 2.0114 68.3628 43.1511 29.2499 2.1869 2.1839 2.17722.1792 68.3371 3.5819 32.5092 3.5791 3.5785 3.5790 3.5792 68.4042 42.6414 2.7339 2.72572.7235 2.7233 2.7229

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

```
ans =  68.3813 \quad 23.0710 \quad 11.2819 \quad 5.4114 \quad 2.8375 \quad 2.8378 \quad 2.8388
```

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans = 0.0292 \quad 18.0009 \quad 13.7414 \quad 7.8576 \quad 0.6220 \quad 0.6214 \quad 0.6214
```

3.9 predict_envmean

Perform estimation of the multivariate mean or prediction for a new observation.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
PredictOutput = predict envmean(ModelOutput, infType)
```

Input

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

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 estimated multivariate mean or the prediction value. A p dimensional column vector.
- PredictOutput.covMatrix: The covariance matrix of PredictOutput.value. A p by p matrix.
- PredictOutput.SE: The standard error of elements in PredictOutput.value. A p dimensional column vector.

Description

If the inference type is prediction, this function predicts a new observation and gives its covariance matrix and standard errors of its elements. If the inference type is estimation, this function gives the estimation of the multivariate mean, its covariance matrix and standard errors of its elements.

```
load Adopted
Y = Adopted(:, 1 : 6);
u = bic_envmean(Y);
ModelOutput = envmean(Y, u);
PredictOutput = predict envmean(ModelOutput, 'prediction')
```

PredictOutput =

value: [6x1 double] covMatrix: [6x6 double] SE: [6x1 double]

${\bf PredictOutput.value}$

ans =

12.3258

85.9841

115.5767

112.1291

114.4862

106.4240

${\bf PredictOutput.SE}$

ans =

2.9090

15.4745

13.4943

13.0308

13.6857

15.4172

3.10 testcoefficient envmean

This function tests the null hypothesis L * mu = A versus the alternative hypothesis L * mu = A, where mu is the multivariate mean.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

- TestInput.L: The matrix multiplied to μ on the left. It is a d1 by p matrix, while d1 is less than or equal to p. Default value: identity matrix I_p .
- TestInput.A: The vector on the right hand side of the equation. It is a d1 dimensional column vector. Default value: d1 by d2 zero matrix.

Output

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

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of L μ . A d1 dimensional column vector.

Description

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

envseq

4.1 bstrp_envseq

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
bootse = bstrp_envseq(X, Y, u, B)
bootse = bstrp_envseq(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 parameters. If one or several (even all) fields are not defined, the default settings are used.

• Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in β 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. The envelope model is applied for the reduction on X, using a sequential algorithm.

```
load Rohwer
     X = Rohwer(:, 4:5);
     Y = Rohwer(:, 1 : 3);
     m = 5;
     u = mfoldcv\_envseq(X, Y, m)
u =
   1
     B = 100;
     bootse = bstrp\_envseq(X, Y, u, B)
bootse =
  0.8738
           0.6855
  0.5191
           0.4404
   0.0961
           0.0654
```

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4.2 envseq

Fit the envelope model using a sequential algorithm.

Contents

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

Syntax

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

Input

X: Predictors. An n by p matrix, p is the number of predictors. The predictors can be univariate or multivariate, discrete or continuous.

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

u: Dimension of the envelope. An integer between 0 and (m-1) * n /m-1.

Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients β . 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 β with respect to Gamma. A u by p matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. A u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r-u by r-u matrix.
- ModelOutput.alpha: The estimated intercept in the envelope model. An r by 1 vector.
- ModelOutput.paramNum: 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

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

Example

```
load Rohwer
    X = Rohwer(:, 4:5);
    Y = Rohwer(:, 1:3);
    m = 5;
    u = mfoldcv envseq(X, Y, m)
u =
   1
    ModelOutput = envseq(X, Y, u)
ModelOutput =
     beta: [3x2 double]
    Sigma: [3x3 double]
    Gamma: [3x1 double]
    Gamma0: [3x2 double]
      eta: [2.5708 1.1966]
    Omega: 752.8146
    Omega0: [2x2 double]
    alpha: [3x1 double]
  paramNum: 11
       n: 69
    ModelOutput.Sigma
ans =
 587.2575 229.9647 37.2716
 229.9647 421.1372 42.9256
```

37.2716 42.9256 12.2696

4.3 mfoldcv_envseq

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
SelectOutput = mfoldcv_envseq(X, Y, m)
SelectOutput = mfoldcv_envseq(X, Y, m, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations.

Y: Responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and r.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
 \begin{split} & \text{load Rohwer} \\ & X = \text{Rohwer}(:,\,4:5); \\ & Y = \text{Rohwer}(:,\,1:3); \\ & \text{Opts.table} = 1;\,\% \text{ Print out the table of average prediction error for each u} \\ & \text{SelectOutput} = \text{mfoldev\_envseq}(X,\,Y,\,5,\,\text{Opts}); \end{split}
```

0 35.575 1 33.713 2 34.352 3 33.823	u	CV error	
	2	33.713 34.352	

SelectOutput.u

```
ans =

1

Opts.perm = 10; % Run 5-fold CV on 10 permutations
Opts.seed = 3; % Set seed for the permutations
Opts.table = 1;
SelectOutput = mfolder envseq(X, Y, 5, Opts);
```

u	CV error
0 1 2 3	34.721 33.190 33.764 33.314

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to \mathbf{u} .

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SelectOutput.PreErr

```
ans =
  34.3525
           32.8549
                    33.3868 32.9159
  34.8898
           33.2683
                    34.4169
                             33.3090
  34.5545
           33.5600
                    34.1334
                             33.7670
  34.8090
           33.2963
                    33.9307
                              33.3307
  34.6288
           33.3523
                    33.6383
                              33.4140
  34.8314
           32.9893
                    33.5988
                             33.0860
  34.8499
                    33.5392
           33.0738
                              33.2285
  34.9425
           33.4004
                    33.7077
                             33.4434
  34.6249 32.9303
                    33.4134
                             33.3155
  34.7250 \quad 33.1717 \quad 33.8734 \quad 33.3336
```

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

```
ans = 34.7208 \quad 33.1897 \quad 33.7638 \quad 33.3144
```

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans = 0.1812 \quad 0.2258 \quad 0.3274 \quad 0.2237
```

henv

5.1 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.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

5.1. AIC_HENV 75

Description

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

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

5.2 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.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. 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.

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Example

$$\begin{aligned} & load\ waterstrider.mat \\ & u = bic_henv(X,\,Y) \end{aligned}$$

 $\mathbf{u} =$

4

5.3 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.

- **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 parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in β 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.

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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

5.4 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 (2013) by using maximum likelihood estimation. This function is the derivative of the objective function.

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5.5 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 (2013) 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.

5.6 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.

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

Opts: A list containing the optional input parameters, 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 to print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the heteroscedastic envelope subspace. An r by u matrix. Default value is the one generated by function get_Init4henv.

Output

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

- ModelOutput.mu: The heteroscedastic envelope estimator of the grand mean. A r by 1 vector.
- ModelOutput.mug: The heteroscedastic envelope estimator of the group mean. A r by p matrix, the ith column of the matrix contains the mean for the ith group.
- ModelOutput.Yfit: A n by r matrix, the ith row gives the group mean of the group that the ith observation belongs to. As X is just a group indicator, and is not ordinal, ModelOutput.mug alone does not tell which group corresponds to which group mean.

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

- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. An r by r-u semi-orthogonal matrix.
- ModelOutput.beta: The heteroscedastic envelope estimator of the group main effect. An r by p matrix, the ith column of the matrix contains the main effect for the ith group.
- ModelOutput.groupInd: A matrix containing the unique values of group indicators. The matrix has p rows. The group mean of the ith row is stored in the ith column of ModelOutput.mug.
- ModelOutput.Sigma: The heteroscedastic envelope estimator of the error covariance matrix. A three dimensional matrix with dimension r, r and p, ModelOutput.Sigma(:, :, i) contains the estimated covariance matrix for the ith group.
- ModelOutput.eta: The coordinates of β with respect to Gamma. A 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. A 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.paramNum: 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.asySE: The asymptotic standard errors for elements in β 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 (2013). When the dimension is r, then the envelope model degenerates to the standard multivariate linear model for comparing group means. When the dimension is 0, it means there is not any group effect, and the fitting is different.

References

- 1. The codes are implemented based on the algorithm in Section 2.2 of Su and Cook (2013).
- 2. The Grassmann manifold optimization step calls the package sg_min 2.4.3 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 (2013).

```
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]
   paramNum: 98
        l: 1.0051e+03
   covMatrix: [32x32 double]
     asySE: [8x3 double]
     ratio: [8x3 double]
       ng: [3x1 double]
ans =
   6.2553 10.8792
                   6.2856
   4.4358 \quad 5.0351
                    4.6347
   4.1925
           4.7967
                    4.2595
   4.5553 \quad 5.9242
                    5.0582
   7.6349 12.1591
                    9.1945
  9.0979 11.1701 10.9407
  11.2834 15.0924 12.0360
   6.6312 10.7068
                    9.7542
```

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5.7 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

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

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.

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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. 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 α .

```
\begin{aligned} & load\ waterstrider.mat \\ & u = lrt\_henv(X,\,Y,\,0.01) \end{aligned} u = 6
```

5.8 mfoldcv henv

Use m-fold cross validation to select the dimension of the envelope subspace for heteroscedastic envelope model.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{aligned} & SelectOutput = mfoldcv\_henv(X, Y, m) \\ & SelectOutput = mfoldcv\_henv(X, Y, m, Opts) \end{aligned}
```

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.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and r.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
load wheatprotein.txt Opts.table = 1; % Print out the table of average prediction error for each u SelectOutput = mfoldcv\_henv(X, Y, 5, Opts);
```

u	CV error
0	1.177
1	1.173
2	1.171

SelectOutput.u

```
ans =

2

Opts.perm = 10; % Run 5-fold CV on 10 permutations
Opts.seed = 3; % Set seed for the permutations
Opts.table = 1;
SelectOutput = mfolder henv(X, Y, 5, Opts);
```

u	CV error
0 1 2	1.088 1.083 1.081

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

SelectOutput.PreErr

ans =

```
1.0746
        1.0704
                 1.0681
1.0921
        1.0881
                 1.0852
1.0849
        1.0803
                 1.0789
1.1077
        1.1037
                 1.1015
1.0795
        1.0756
                 1.0732
1.0908
        1.0861
                 1.0843
1.0921
        1.0880
                 1.0865
1.0845
        1.0809
                 1.0776
1.0815
        1.0769
                 1.0756
1.0878
        1.0838
                  1.0815
```

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

```
ans = 1.0876 \quad 1.0834 \quad 1.0812
```

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans = 0.0091 \quad 0.0091 \quad 0.0091
```

5.9 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
        0
   1
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
           0.3753 \quad 0.3735
           0.3271
  0.3467
                    0.3179
  -0.1954 -0.2100 -0.3488
Xnew =
    1
   0
     PredictOutput = predict_henv(ModelOutput, Xnew, 'estimation')
     PredictOutput.value %This is the 3rd group mean
     {\bf 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
```

```
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
  0.3854
```

5.10 testcoefficient henv

This function tests the null hypothesis L^* beta *R = A versus the alternative hypothesis L^* beta *R = 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 β 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 β 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 β sum to 0. Then we cannot use I_p as default.
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

Output

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

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

Description

This function tests for hypothesis $H_0: L\beta R = A$, versus $H_\alpha: L\beta R \neq A$. The β 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.

```
\begin{split} & load\ waterstrider.mat \\ & u = lrt\_henv(X,\,Y,\,0.01); \\ & ModelOutput = henv(X,\,Y,\,u); \\ & TestOutout = testcoefficient\_henv(ModelOutput); \end{split}
```

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

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

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

ienv

6.1 aic_ienv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = aic_ienv(X, Y)

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is the number of observations. The predictors can be univariate or multivariate, discrete or continuous.

Y: Multivariate responses. An n by r matrix, r is the number of responses. The responses must be continuous variables.

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

Description

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

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

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6.2 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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. 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}
```

 $\mathbf{u} =$

1

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6.3 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.

B: Number of bootstrap samples. A positive integer.

Opts: A list containing the optional input parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in β 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)
```

```
u =
```

1

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

bootse =

13.4695 4.9601 7.4709 2.7315 14.9316 5.2913 8.7597 3.0853 6.4. DF4IENV 101

6.4 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.

6.5 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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6.6 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.

Opts: A list containing the optional input parameters, 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 to print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the inner envelope subspace. An r by u matrix. Default value is the one generated by function get_Init.

Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients β . 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 β with respect to Gamma1. A 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 β with respect to Gamma0. A p by (p-u) matrix.
- ModelOutput.Omega1: The coordinates of Sigma with respect to Gamma1. A 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.asySE: Asymptotic standard error for elements in β 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 β . An r by p matrix.
- ModelOutput.paramNum: The number of parameters in the inner envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

Description

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

References

- 1. The codes are implemented based on the algorithm in Su and Cook (2012).
- 2. The Grassmann manifold optimization step calls the package sg_min 2.4.3 by Ross Lippert (http://web.mit.edu/~ripper/www/sgmin.html).

Example

1

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

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

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

ModelOutput =

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

ans =

0.0035 0.2111 0.0166 0.0940 -0.0062 0.1322 0.0044 0.0178

6.7 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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. Logical 0 or 1. Default value: 0.

Output

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

Description

This function implements the likelihood ratio testing procedure to select the dimension of the inner envelope subspace, with pre-specified significance level α .

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

6.8 mfoldcv ienv

Select the dimension of the inner envelope subspace using m-fold cross validation.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
SelectOutput = mfoldcv_ienv(X, Y, m)
SelectOutput = mfoldcv_ienv(X, Y, m, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations.

Y: Responses. An n by r matrix, r is the number of responses. The number of the responses should be greater than the number of the predictors. And they must be continuous variables.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the inner envelope subspace selected by m-fold cross validation. An integer between 0 and p.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
load irisf.mat Opts.table = 1; \% Print out the table of average prediction error for each u SelectOutput = mfoldcv ienv(X, Y, 5, Opts);
```

u	CV error
0 1 2	7.869 12.865 13.068
_	10.000

SelectOutput.u

```
ans = 0
```

```
\begin{aligned} & \text{Opts.perm} = 10; \% \text{ Run 5-fold CV on 10 permutations} \\ & \text{Opts.seed} = 3; \% \text{ Set seed for the permutations} \\ & \text{Opts.table} = 1; \\ & \text{SelectOutput} = \text{mfoldcv\_ienv}(X, Y, 5, \text{Opts}); \end{aligned}
```

u	CV error
0	7.871
1	13.987
2	8.660

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

SelectOutput.PreErr

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```
7.8658 \quad \  8.0292 \quad 10.2529
7.8439 \quad 15.3317
                   9.1913
7.8063 14.3470
                   7.9989
7.8566 \quad 16.2194
                   8.0552
7.8660 14.7267
                   8.0347
7.8460 17.5724
                   9.5129
7.8152 \quad 14.2335
                   8.0367
7.9323 8.2747
                   8.1148
7.8682 14.9348
                   8.0369
8.0062 16.1967
                   9.3622
```

ans =

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

```
ans = 7.8707 \quad 13.9866 \quad 8.6596
```

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans = 0.0587 \quad 3.2368 \quad 0.8372
```

6.9 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}
```

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```
PredictOutput = \\
      value: [4x1 double]
   covMatrix: [4x4 double]
        SE: [4x1 double]
ans =
  49.9458 \quad 51.0000
  34.2592 \quad 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
```

6.10 testcoefficient ienv

This function tests the null hypothesis L^* beta *R = A versus the alternative hypothesis L^* beta *R = 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 β 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 β on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix I_p .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

Output

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

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

Description

This function tests for hypothesis $H_0: L\beta R = A$, versus $H_\alpha: L\beta R \neq A$. The β 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.

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```
\begin{array}{c} load\ irisf.mat\\ d=bic\_ienv(X,Y);\\ ModelOutput=ienv(X,Y,d);\\ TestOutout=testcoefficient\_ienv(ModelOutput);\\ \\ \hline Test\ Hypothesis & Chisq\ Statistic & DF & P-value\\ \hline \\ L*beta*R=A & 4642.913 & 8 & 0.0000\\ \hline \\ \hline TestInput.L=rand(2,4);\\ TestInput.R=rand(2,1);\\ TestInput.A=zeros(2,1);\\ TestOutout=testcoefficient\_ienv(ModelOutput, TestInput);\\ \\ \hline Test\ Hypothesis & Chisq\ Statistic & DF & P-value\\ \hline \\ L*beta*R=A & 1834.229 & 2 & 0.0000\\ \hline \end{array}
```

penv

7.1 aic_penv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{split} u &= aic\_penv(X, \, Y) \\ u &= aic\_penv(X, \, Y, \, Opts) \end{split}
```

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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

Description

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

```
\begin{aligned} & \text{load fiberpaper.dat} \\ & Y = \text{fiberpaper}(:, 1:4); \\ & X.X1 = \text{fiberpaper}(:, 7); \\ & X.X2 = \text{fiberpaper}(:, 5:6); \\ & u = \text{aic\_penv}(X, Y) \end{aligned}
```

7.2. BIC_PENV 117

7.2 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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. 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.

```
\begin{array}{c} \operatorname{load\ fiberpaper.dat} \\ Y = \operatorname{fiberpaper}(:,\,1:4); \\ X.X1 = \operatorname{fiberpaper}(:,\,7); \\ X.X2 = \operatorname{fiberpaper}(:,\,5:6); \\ u = \operatorname{bic\_penv}(X,\,Y) \end{array}
```

7.3. BSTRP_PENV 119

7.3 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 parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in β_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.

```
\begin{aligned} & \text{load fiberpaper.dat} \\ & Y = \text{fiberpaper}(:,\,1:4); \\ & X.X1 = \text{fiberpaper}(:,\,7); \\ & X.X2 = \text{fiberpaper}(:,\,5:6); \\ & \text{alpha} = 0.01; \\ & u = \text{modelselectlrt}(X,\,Y,\,\text{alpha},\,\text{'penv'}) \end{aligned} u = \\ 1 \\ & B = 100; \\ & \text{bootse} = \text{bstrp\_penv}(X,\,Y,\,u,\,B) \end{aligned} bootse = \\ & 0.0074 \\ & 0.0021 \\ & 0.0043 \\ & 0.0019 \end{aligned}
```

7.4. LRT_PENV 121

7.4 lrt_penv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = lrt\_penv(X, Y, alpha)

u = lrt\_penv(X, Y, alpha, Opts)
```

Input

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

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

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

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

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. 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 α .

```
\begin{aligned} & \text{load fiberpaper.dat} \\ & Y = \text{fiberpaper}(:, 1:4); \\ & X.X1 = \text{fiberpaper}(:, 7); \\ & X.X2 = \text{fiberpaper}(:, 5:6); \\ & \text{alpha} = 0.01; \\ & u = \text{lrt\_penv}(X, Y, \text{alpha}) \end{aligned}
```

7.5 mfoldcv_penv

Select the dimension of the partial envelope subspace using m-fold cross validation.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{split} & SelectOutput = mfoldcv\_penv(X, \, Y, \, m) \\ & SelectOutput = mfoldcv\_penv(X, \, Y, \, m, \, Opts) \end{split}
```

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.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value:
 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the partial envelope subspace selected by m-fold cross validation. An integer between 0 and r.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
load fiberpaper.dat Y = \text{fiberpaper}(:, 1:4); X.X1 = \text{fiberpaper}(:, 7); X.X2 = \text{fiberpaper}(:, 5:6); Opts.table = 1; \% \text{ Print out the table of average prediction error for each u SelectOutput} = \text{mfoldev\_penv}(X, Y, 5, Opts);}
```

u	CV error
0	3.384
1	4.423
2	4.485
3	3.471
4	4.486

SelectOutput.u

```
ans = 0 Opts.perm = 10; % Run 5-fold CV on 10 permutations Opts.seed = 3; % Set seed for the permutations Opts.table = 1; SelectOutput = mfoldcv_penv(X, Y, 5, Opts);
```

u	CV error
0	2.416
1	2.410
2	2.400
3	2.493
	100
4	2.513

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

${\bf SelectOutput. Pre Err}$

ans =				
2.3928	2.3917	2.4230	2.4304	2.4584
2.4007	2.4007	2.4873	2.4312	2.4871
2.3040	2.3031	2.3598	2.3176	2.3747
2.3118	2.3103	2.3880	2.3786	2.3875
2.4937	2.4927	2.5157	2.5055	2.5149
2.3756	2.3756	2.3892	2.3851	2.3883
2.4432	2.6921	2.6902	2.7041	2.7020
2.5305	2.5286	2.5467	2.5416	2.5595
2.4482	2.6476	2.6520	2.6662	2.6648
2.4580	2.4568	2.5684	2.5677	2.5933

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

```
ans =  2.4159 \quad 2.4599 \quad 2.5020 \quad 2.4928 \quad 2.5130
```

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans =  0.0734 \quad 0.1322 \quad 0.1140 \quad 0.1273 \quad 0.1162
```

7.6 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.

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

Opts: A list containing the optional input parameters, 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 to print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the partial envelope subspace. An r by u matrix. Default value is the one generated by function get_Init.

Output

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

- ModelOutput.beta1: The partial envelope estimator of β_1 , which is the regression coefficients for X1. An r by p1 matrix.
- ModelOutput.beta2: The partial envelope estimator of β_2 , which is the regression coefficients for X2. An r by p2 matrix.

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

- ModelOutput.Gamma: The orthogonal basis of the partial envelope subspace. An r by u semi-orthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the partial envelope subspace. An r by r u semi-orthogonal matrix.
- ModelOutput.eta: The coordinates of β_1 with respect to Gamma. A u by p1 matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. A 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.asySE: Asymptotic standard error for elements in β_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 β_1 . An r by p1 matrix.
- ModelOutput.paramNum: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

Description

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

References

- 1. The codes are implemented based on the algorithm in Section 3.2 of Su and Cook (2012).
- 2. The Grassmann manifold optimization step calls the package sg_min 2.4.3 by Ross Lippert (http://web.mit.edu/~ripper/www/sgmin.html).

Example

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

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
X.X1 = fiberpaper(:, 7);
X.X2 = fiberpaper(:, 5 : 6);
alpha = 0.01;
u = modelselectlrt(X, Y, alpha, 'penv')
```

```
u =
   1
     ModelOutput = penv(X, Y, u)
     {\bf Model Output. Omega}
     eig(ModelOutput.Omega0)
     ModelOutput.ratio
ModelOutput =
     beta1: [4x1 double]
     beta2: [4x2 double]
     alpha: [4x1 double]
     Gamma: [4x1 double]
       eta: 0.0047
     Omega: 0.0149
     Omega0: [3x3 double]
     Sigma: [4x4 double]
        1: -35.6323
   paramNum: 23
   covMatrix: [12x12 double]
     asySE: [4x1 double]
     ratio: [4x1 double]
        n: 62
ans =
   0.0149
ans =
   4.9819
   0.0999
   0.0050
ans =
  65.9692
  6.8217
  10.4152
  9.6228
```

7.7 predict_penv

Perform estimation or prediction under the partial envelope model.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

PredictOutput = predict_penv(ModelOutput, Xnew, infType)

Input

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

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

- * Xnew.X1: A p1 by 1 vector containing the value of X1.
- * Xnew.X2: A p2 by 1 vector containing the value of X2.

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

Output

PredictOutput: A list containing the results of the inference.

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

Description

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

```
load fiberpaper.dat
     Y = fiberpaper(:, 1 : 4);
     X.X1 = fiberpaper(:, 7);
     X.X2 = fiberpaper(:, 5:6);
     alpha = 0.01;
     u = modelselectlrt(X, Y, alpha, 'penv');
     ModelOutput = penv(X, Y, u);
     Xnew.X1 = X.X1(1, :);
     Xnew.X2 = X.X2(1, :);
     PredictOutput = predict penv(ModelOutput, Xnew, 'estimation')
     [PredictOutput.value, Y(1, :)] % Compare the fitted value with the data
     PredictOutput.SE
PredictOutput =
      value: [4x1 double]
   covMatrix: [4x4 double]
        SE: [4x1 double]
ans =
  21.1169 \quad 21.3120
   7.1173 7.0390
  5.3637 \quad 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

7.8 testcoefficient_penv

This function tests the null hypothesis L * beta1 * R = A versus the alternative hypothesis L * beta1 * R = 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 β_1 on the left. It is a d1 by r matrix, while d1 is less than or equal to r. Default value: identity matrix I_r .
- TestInput.R: The matrix multiplied to β_1 on the right. It is a p1 by d2 matrix, while d2 is less than or equal to p1. Default value: identity matrix I_{p1} .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

Output

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

- TestOutput.chisqStatistic: The test statistics. A real number.
- TestOutput.df: The degrees of freedom of the reference chi-squared distribution. A positive integer.
- TestOutput.pValue: p-value of the test. A real number in [0, 1].
- TestOutput.covMatrix: The covariance matrix of $vec(L\beta_1 R)$. A d1 * d2 by d1 * d2 matrix.

Description

This function tests for hypothesis $H_0: L\beta_1R = A$, versus $H_\alpha: L\beta_1R \neq A$. The β_1 is estimated by the partial envelope model. If the user does not specify the values for L, R and A, then the test is equivalent to the standard F test on if $\beta_1 = 0$. The test statistics used is vec $(L\beta_1R - A)$ $\hat{\Sigma}^{-1}$ vec $(L\beta_1R - A)^T$, and the reference distribution is chi-squared distribution with degrees of freedom d1 * d2.

Example

```
load fiberpaper.dat
    Y = fiberpaper(:, 1 : 4);
    X.X1 = fiberpaper(:, 7);
    X.X2 = fiberpaper(:, 5:6);
    alpha = 0.01;
    u = modelselectlrt(X, Y, alpha, 'penv');
    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

8.1 aic_senv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{split} u &= aic\_senv(X, \, Y) \\ u &= aic\_senv(X, \, Y, \, Opts) \end{split}
```

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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value:
 0.
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.
- Opts.rep: Number of replicates for scales. This option imposes special structure on scaling parameters. For example, if Opts.rep = [3 4], this means that the first three responses have the same scale and the next four responses share a different scale. The elements of this vector should sum to r. If not specified, the default is [], then all responses will be scaled differently. If all responses have the same scale, input [r], then the regular envelope will be applied to the data. The input should be a row vector.

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Output

 $\boldsymbol{u}\text{:}$ Dimension of the scaled 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.

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

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8.2 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 parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. Logical 0 or 1. Default value: 0.
- Opts.rep: Number of replicates for scales. This option imposes special structure on scaling parameters. For example, if Opts.rep = [3 4], this means that the first three responses have the same scale and the next four responses share a different scale. The elements of this vector should sum to r. If not specified, the default is [], then all responses will be scaled differently. If all responses have the same scale, input [r], then the regular envelope will be applied to the data. The input should be a row vector.

Output

u: Dimension of the scaled 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.

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Example

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

 $\mathbf{u} =$

2

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8.3 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.

 ${f u}$: 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 parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.
- Opts.rep: Number of replicates for scales. This option imposes special structure on scaling parameters. For example, if Opts.rep = [3 4], this means that the first three responses have the same scale and the next four responses share a different scale. The elements of this vector should sum to r. If not specified, the default is [], then all responses will be scaled differently. If all responses have the same scale, input [r], then the regular envelope will be applied to the data. The input should be a row vector.

Output

bootse: The standard error for elements in β 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.

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```
load('sales.txt')
     Y = sales(:, 4:7);
     X = sales(:, 1:3);
     u = bic\_senv(X, \, Y)
u =
   2
     B = 20;
     bootse = bstrp\_senv(X,\,Y,\,u,\,B)
bootse =
   0.0539
            0.0472 \quad 0.0554
   0.0675
            0.0912
                     0.1178
   0.0567
            0.0781
                     0.0791
   0.0986
            0.0944
                     0.1283
```

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8.4 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.

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8.5 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 (2013) using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace.

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8.6 mfoldcv senv

Select the dimension of the scaled envelope subspace using m-fold cross validation.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
SelectOutput = mfoldcv_senv(X, Y, m)
SelectOutput = mfoldcv_senv(X, Y, m, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations.

Y: Responses. An n by r matrix, r is the number of responses. The number of the responses should be greater than the number of the predictors. And they must be continuous variables.

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.rep: Number of replicates for scales. This option imposes special structure on scaling parameters. For example, if Opts.rep = [3 4], this means that the first three responses have the same scale and the next four responses share a different scale. The elements of this vector should sum to r. If not specified, the default is [], then all responses will be scaled differently. If all responses have the same scale, input [r], then the regular envelope will be applied to the data. The input should be a row vector.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the scaled envelope subspace selected by m-fold cross validation. An integer between 0 and r.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
\begin{aligned} & load('sales.txt') \\ & Y = sales(:, 4:7); \\ & X = sales(:, 1:3); \\ & Opts.table = 1; \% \ Print \ out \ the \ table \ of \ average \ prediction \ error \ for \ each \ u \\ & SelectOutput = mfoldcv \ senv(X, Y, 5, Opts); \end{aligned}
```

u	CV error
0 1 2 3 4	11.969 5.750 5.266 5.410 5.343

SelectOutput.u

```
ans =

2

Opts.perm = 10; % Run 5-fold CV on 10 permutations
Opts.seed = 3; % Set seed for the permutations
Opts.table = 1;
SelectOutput = mfoldcv_senv(X, Y, 5, Opts);
```

u	CV error
0	11.977
1	5.754
2	5.305
3	5.465
4	5.437

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

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${\bf SelectOutput.PreErr}$

```
ans =
  11.9619
            5.7170
                     5.2153
                              5.4024
                                       5.3363
  12.1588
            5.6580
                     5.1543
                              5.2932
                                       5.3016
  11.9315
            5.8612
                     5.3559
                              5.5420
                                       5.5057
  11.9389
            5.7846
                     5.3054
                              5.5447
                                       5.4539
  11.9335
            5.8343
                     5.3847
                              5.9421
                                       5.9300
  11.8577
            5.6179
                     5.2153
                              5.3673
                                       5.3689
  11.9126
            5.7536
                     5.2937
                              5.2898
                                       5.3091
  12.2099
            5.7924
                     5.3580
                              5.3046
                                       5.2770
  11.9684
            5.8209
                     5.4442
                              5.4736
                                       5.4700
  11.9016
            5.6978
                     5.3260
                              5.4891
                                       5.4158
```

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

std(SelectOutput.PreErr) % Compute the standard deviations of the prediction errors for each u

```
ans = 0.1141 \quad 0.0796 \quad 0.0885 \quad 0.1944 \quad 0.1899
```

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8.7 objfun

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

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

Input

d: An r - 1 dimensional column vector containing the scales for the 2nd to the rth responses. All the entries in d are positive.

Gamma: A r by u semi-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 Cook and Su (2013) using maximum likelihood estimation.

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8.8 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}(\text{'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} \quad \operatorname{senv}(\operatorname{ModelOutput}, \operatorname{Xnew}, \operatorname{'estimation'}) \end{split}
```

[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 \quad 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')
     {\bf 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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8.9 **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 parameters, 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 to print out number of iterations, logical 0 or 1. Default value: 0.
- Opts.rep: Number of replicates for scales. This option imposes special structure on scaling parameters. For example, if Opts.rep = [3 4], this means that the first three responses have the same scale and the next four responses share a different scale. The elements of this vector should sum to r. If not specified, the default is [], then all responses will be scaled differently. If all responses have the same scale, input [r], then the regular envelope will be applied to the data. The input should be a row vector.

Output

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

- ModelOutput.beta: The scaled envelope estimator of the regression coefficients β . 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.

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• 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 β with respect to Gamma. A u by p matrix.
- ModelOutput.Omega: The coordinates of Sigma with respect to Gamma. A u by u matrix.
- ModelOutput.Omega0: The coordinates of Sigma with respect to Gamma0. An r u by r
 - u matrix.
- ModelOutput.alpha: The estimated intercept in the scaled envelope model. An r by 1 vector.
- ModelOutput.l: The maximized log likelihood function. A real number.
- ModelOutput.covMatrix: The asymptotic covariance of vec(β). An rp by rp matrix. The
 covariance matrix returned are asymptotic. For the actual standard errors, multiply by 1
 / n.
- ModelOutput.asySE: Asymptotic standard error for elements in β 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 β . An r by p matrix.
- ModelOutput.paramNum: 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 (2013). When the dimension is r, then the scaled envelope model degenerates to the standard multivariate linear regression. When the dimension is 0, it means that r and r are uncorrelated, and the fitting is different.

References

- 1. The codes are implemented based on the algorithm in Section 4.1 of Cook and Su (2013).
- 2. The Grassmann manifold optimization step calls the package sg_min 2.4.3 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 (2013).

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

11 =

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ModelOutput = senv(X, Y, u)

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]
paramNum: 23
l: -386.1900
covMatrix: [12x12 double]
asySE: [4x3 double]
ratio: [4x3 double]
n: 50

Model Output. Lambda

ans =

1.0000	0	0	0
0	0.9729	0	0
0	0	0.8067	0
0	0	0	1 7016

1 - 1 ./ ModelOutput.ratio

ans =

0.6823	0.4901	0.6287
0.6119	0.3188	0.5594
0.4036	0.1267	0.3484
0.5329	0.4585	0.5180

This example demonstrates the use of opts.rep. In this example, the first six responses are measured in mg/ml, and the next responses are measured in ug/ml.

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```
\begin{aligned} & load('Urine.txt') \\ & Y = Urine(:, 3:11); \\ & X = Urine(:, 12:14); \\ & Opts.rep = [6 \ 3]; \\ & u = bic\_senv(X, Y, Opts) \end{aligned} u = \\ & 1 ModelOutput = senv(X, Y, u, Opts)
```

${\bf ModelOutput} =$

beta: [9x3 double]
Sigma: [9x9 double]
Lambda: [9x9 double]
Gamma: [9x1 double]
Gamma0: [9x8 double]
eta: [0.1064 0.1326 0.1465]
Omega: 0.0043
Omega0: [8x8 double]
alpha: [9x1 double]
paramNum: 58
l: -500.3789
covMatrix: [27x27 double]
asySE: [9x3 double]
ratio: [9x3 double]
n: 45

ModelOutput.Lambda

ans =

1.0000	0	0	0	0	0	0	0	0
0	1.0000	0	0	0	0	0	0	0
0	0	1.0000	0	0	0	0	0	0
0	0	0	1.0000	0	0	0	0	0
0	0	0	0	1.0000	0	0	0	0
0	0	0	0	0	1.0000	0	0	0
0	0	0	0	0	0	0.4356	0	0
0	0	0	0	0	0	0	0.4356	0
0	0	0	0	0	0	0	0	0.4356

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8.10 testcoefficient senv

This function tests the null hypothesis L^* beta *R = A versus the alternative hypothesis L^* beta *R = 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 β 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 β on the right. It is a p by d2 matrix, while d2 is less than or equal to p. Default value: identity matrix I_p .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

Output

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

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

Description

This function tests for hypothesis $H_0: L\beta R = A$, versus $H_\alpha: L\beta R \neq A$. The β 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.

```
\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	4660.161	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

9.1 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 and n is number of observations. The predictors must be continuous variables.

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

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains AIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

9.1. AIC_XENV 155

Description

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

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

9.2 bic xenv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

u = bic\_xenv(X, Y, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains BIC and log likelihood for each u. Logical 0 or 1. Default value: 0.

Output

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

Description

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

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

9.2. BIC_XENV 157

 $\mathbf{u} =$

4

9.3 bstrp_xenv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

Opts: A list containing the optional input parameters, 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 to print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

bootse: The standard error for elements in β computed by bootstrap. A p by r matrix.

Description

This function computes the bootstrap standard errors for the regression coefficients in the envelope model by bootstrapping the (X, Y) jointly. The envelope model here is for the reduction on X.

9.3. BSTRP_XENV 159

```
load\ wheat protein.txt
     X = wheatprotein(:, 1:6);
     Y = wheatprotein(:, 7);
      alpha = 0.01;
     u = \mathrm{lrt} \_\mathrm{xenv}(X,\,Y,\,\mathrm{alpha})
u =
    4
      B = 100;
      bootse = bstrp\_xenv(X, Y, u, B)
bootse =
   0.0385
   0.0915
   0.1007
   0.0268
   0.0039
   0.0203
```

9.4 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: A 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. (2013) by using maximum likelihood estimation. This function is the derivative of the objective function.

9.5. F4XENV 161

9.5 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. (2013) using maximum likelihood estimation. The columns of the semi-orthogonal matrix that minimizes this function span the estimated envelope subspace.

9.6 lrt xenv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = lrt\_xenv(X, Y, alpha)

u = lrt\_xenv(X, Y, alpha, Opts)
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

Opts: A list containing the optional input parameters, 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 to print out dimension selection process. Logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains log likelihood, test statistic, degrees of freedom and p-value for each test. 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 α .

9.6. LRT_XENV 163

```
\begin{aligned} & \text{load wheatprotein.txt} \\ & X = \text{wheatprotein}(:,\,1:6); \\ & Y = \text{wheatprotein}(:,\,7); \\ & \text{alpha} = 0.01; \\ & u = \text{lrt\_xenv}(X,\,Y,\,\text{alpha}) \end{aligned} u = \underbrace{ } \end{aligned}
```

9.7 mfoldcv xenv

Use m-fold cross validation to select the dimension of the envelope subspace for the reduction on X.

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
\begin{aligned} & SelectOutput = mfoldcv\_xenv(X, Y, m) \\ & SelectOutput = mfoldcv\_xenv(X, Y, m, Opts) \end{aligned}
```

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value: 0.
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and p.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
load wheatprotein.txt

X = wheatprotein(:, 1 : 6);

Y = wheatprotein(:, 7);

Opts.table = 1; % Print out the table of average prediction error for each u

SelectOutput = mfoldcv xenv(X, Y, 5, Opts);
```

u	CV error
0	1.474
1	0.281
2	0.271
3	0.288
4	0.219
5	0.221
6	0.221

SelectOutput.u

```
ans =

4

Opts.perm = 10; % Run 5-fold CV on 10 permutations
Opts.seed = 3; % Set seed for the permutations
Opts.table = 1;
SelectOutput = mfoldcv_xenv(X, Y, 5, Opts);
```

u	CV error
0	1.473
1	0.274
2	0.273
3	0.283
4	0.234
5	0.214

```
6 0.214
```

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

${\bf SelectOutput.PreErr}$

a	ns =						
	1.4825	0.2751	0.2748	0.2933	0.2273	0.2265	0.2265
	1.4807	0.3163	0.3178	0.3178	0.2394	0.2398	0.2391
	1.4686	0.2592	0.2585	0.2574	0.2207	0.2005	0.2006
	1.4705	0.2530	0.2523	0.2699	0.1984	0.1972	0.1972
	1.4658	0.3015	0.2941	0.3082	0.2232	0.2226	0.2221
	1.4698	0.2525	0.2528	0.2511	0.2536	0.2237	0.2241
	1.4656	0.2589	0.2589	0.2813	0.2648	0.2077	0.2077
	1.4730	0.2833	0.2829	0.2988	0.2252	0.2174	0.2166
	1.4896	0.2842	0.2845	0.3074	0.2825	0.1993	0.1993
	1.4609	0.2548	0.2545	0.2474	0.2032	0.2028	0.2027

 $\operatorname{mean}(\operatorname{SelectOutput.PreErr})~\%$ Compute the average of prediction errors for each u

 $std(SelectOutput.PreErr)\ \%\ Compute\ the\ standard\ deviations\ of\ the\ prediction\ errors\ for\ each\ u$

```
ans =  0.0089 \quad 0.0223 \quad 0.0218 \quad 0.0256 \quad 0.0265 \quad 0.0143 \quad 0.0142
```

9.8 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.

```
\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 \quad 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
```

9.9 testcoefficient xenv

This function tests the null hypothesis L^* beta *R = A versus the alternative hypothesis L^* beta *R = 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 β on the left. It is a d1 by p matrix, while d1 is less than or equal to p. Default value: identity matrix I_p .
- TestInput.R: The matrix multiplied to β on the right. It is a r by d2 matrix, while d2 is less than or equal to r. Default value: identity matrix I_r .
- TestInput.A: The matrix on the right hand side of the equation. It is a d1 by d2 matrix. Default value: d1 by d2 zero matrix.

Output

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

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

Description

This function tests for hypothesis $H_0: L\beta R = A$, versus $H_\alpha: L\beta R \neq A$. The β 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.

```
 \begin{split} & load\ wheatprotein.txt \\ & X \!\!=\!\! wheatprotein(:,\,1:6); \\ & Y \!\!=\!\! wheatprotein(:,\,7); \\ & u = bic\_xenv(X,\,Y); \\ & ModelOutput \!\!=\!\! xenv(X,\,Y,\,u); \\ & TestOutout = testcoefficient\_xenv(ModelOutput); \end{split}
```

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

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

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

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9.10 xenv

Fit the envelope model for the reduction on X.

Contents

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

Syntax

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

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

Opts: A list containing the optional input parameters, 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 to print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- Opts.init: The initial value for the envelope subspace. A p by u matrix. Default value is the one generated by function get_Init.

Output

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

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

• ModelOutput.Omega0: The coordinates of Σ_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.asySE: Asymptotic standard error for elements in β 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 β . A p by r matrix.
- ModelOutput.paramNum: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

Description

This function fits the envelope model in the predictor's space, using the maximum likelihood estimation. When the dimension of the envelope is between 1 and r - 1, we implemented the algorithm in Cook et al. (2013). When the dimension is r, then the envelope model degenerates to the standard multivariate linear regression. When the dimension is 0, it means that X and Y are uncorrelated, and the fitting is different.

References

- 1. The codes are implemented based on the algorithm in Section 4.5.1 of Cook et al (2013).
- 2. The Grassmann manifold optimization step calls the package sg_min 2.4.3 by Ross Lippert (http://web.mit.edu/~ripper/www/sgmin.html).

```
\label{eq:continuous_signal_condition} \begin{split} & \text{load wheatprotein}(:,1:6); \\ & X = \text{wheatprotein}(:,7); \\ & Y = \text{wheatprotein}(:,7); \\ & p = \text{size}(X,2); \\ & \text{ModelOutput} = \text{xenv}(X,Y,p); \\ & \% \text{ When } u = p, \text{ the envelope model reduces to the ordinary least squares} \\ & \% \text{ regression} \\ & \text{temp} = \text{fit\_OLS}(X,Y); \\ & \text{temp.SigmaOLS} \\ & \text{ModelOutput.sigYcX} \end{split}
```

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```
ans =
  0.0321
ans =
   0.0321
     temp.betaOLS'
     {\bf Model Output. beta}
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)
{\bf 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 l: -865.6407

```
covMatrix: [6x6 double]
      asySE: [6x1 double]
      ratio: [6x1 double]
   paramNum: 27
        n: 50
     \% To compare with the results obtained by Partial Least Squares, use the
     % plsregress command
     [XL,\,YL,\,XS,\,YS,\,BETA,\,PCTVAR,\,MSE,\,stats] = plsregress(X,\,Y,\,u);
     ModelOutput.beta
     BETA(2 : end, :)
ans =
  -0.0443
  -0.0481
  0.3377
  -0.1963
  0.0019
  -0.0487
ans =
  -0.0199
  0.1373
  0.1309
  -0.1827
  0.0056
  -0.0708
```

xenvpls

10.1 bstrp_xenvpls

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

B: Number of bootstrap samples. A positive integer.

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

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

Output

bootse: The standard error for elements in β computed by bootstrap. A p by r matrix.

Description

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

```
\begin{aligned} & load\ VocabGrowth\\ & X = VocabGrowth(:,\,1:3);\\ & Y = VocabGrowth(:,\,4);\\ & m = 5;\\ & u = mfoldcv\_xenvpls(X,\,Y,\,m) \end{aligned} u = 1 1 B = 100;\\ & bootse = bstrp\_xenvpls(X,\,Y,\,u,\,B) bootse = 0.0230\\ & 0.0235\\ & 0.0273 \end{aligned}
```

10.2 mfoldcv_xenvpls

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

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

- Opts.verbose: Flag to print out dimension selection process, logical 0 or 1. Default value:
- Opts.table: Flag to tabulate the results, which contains cross validation error for each u. Logical 0 or 1. Default value: 0.
- Opts.perm: A positive integer indicating number permutations of the observations, m-fold cross validation is run on each permutation. If not specified, the division is based on the sequential order of the observations.
- Opts.seed: A real number that set the seeds for permutations. Default value is 1.

Output

SelectOutput: A list containing the results of the selection.

- SelectOutput.u: The dimension of the envelope subspace selected by m-fold cross validation. An integer between 0 and p.
- SelectOutput.PreErr: A vector containing prediction errors for each u if Opts.perm is not specified, or a matrix with the element in the ith row and jth column containing the prediction error for u=j-1 and ith permutation of the observations.

Description

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

Example

```
 \begin{aligned} & \text{load VocabGrowth} \\ & X = \text{VocabGrowth}(:, 1:3); \\ & Y = \text{VocabGrowth}(:, 4); \\ & \text{Opts.table} = 1; \% \text{ Print out the table of average prediction error for each u} \\ & \text{SelectOutput} = \text{mfoldev} \quad \text{xenvpls}(X, Y, 5, \text{Opts}); \end{aligned}
```

u	CV error
0 1 2 3	1.959 1.091 1.127 1.130

SelectOutput.u

```
ans =  1  Opts.perm = 10; % Run 5-fold CV on 10 permutations Opts.seed = 3; % Set seed for the permutations Opts.table = 1; SelectOutput = mfoldcv_xenvpls(X, Y, 5, Opts);
```

u	CV error
0	1.942
1	1.087
2	1.108
3	1.110

The rows of PreErr corresponds to permutations, and the columns of PreErr corresponds to u.

${\bf SelectOutput.PreErr}$

ans =			
1.9576	1.1076	1.1272	1.1265
1.9500	1.0664	1.0834	1.0856
1.9347	1.0878	1.0938	1.0947
1.9298	1.0747	1.1080	1.1122
1.9309	1.0956	1.1130	1.1187
1.9659	1.0995	1.1180	1.1163
1.9312	1.0920	1.1019	1.1023
1.9188	1.0582	1.0836	1.0850
1.9303	1.0798	1.1009	1.1007
1.9676	1.1114	1.1494	1.1558

mean(SelectOutput.PreErr) % Compute the average of prediction errors for each u

 $\operatorname{std}(\operatorname{SelectOutput.PreErr})$ % Compute the standard deviations of the prediction errors for each u

```
ans =  0.0171 \quad 0.0174 \quad 0.0203 \quad 0.0213
```

10.3 xenvpls

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

Contents

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

Syntax

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The predictors must be continuous variables.

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

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

Output

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

- ModelOutput.beta: The envelope estimator of the regression coefficients β . A p by r matrix
- ModelOutput.SigX: The envelope estimator of the covariance matrix of X, Σ_X . A p by p matrix.
- ModelOutput.Gamma: The orthogonal basis of the envelope subspace. A p by u semiorthogonal matrix.
- ModelOutput.Gamma0: The orthogonal basis of the complement of the envelope subspace. A p by p-u semi-orthogonal matrix.
- ModelOutput.eta: The coordinates of β with respect to Gamma. A u by r matrix.
- Model Output. Omega: The coordinates of Σ_X with respect to Gamma. A u by u matrix.
- Model Output.Omega
0: The coordinates of Σ_X with respect to Gamma
0. 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.paramNum: The number of parameters in the envelope model. A positive integer.
- ModelOutput.n: The number of observations in the data. A positive integer.

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Description

This function fits the envelope model in the predictor's space, by the partial least squares algorithm in Cook et al. (2013). In the population level, this algorithm is equivalent to that in xenv.m, which uses the maximum likelihood estimation. In the sample version, the two algorithms are different. And this algorithm is much faster, which provides a root n consistent starting value for the one in xenv.m.

Reference

The codes are implemented based on the algorithm in Section 4.3 of Cook et al (2013).

Example

```
load VocabGrowth
    X = VocabGrowth(:, 1:3);
    Y = VocabGrowth(:, 4);
    m = 5;
    u = mfoldcv xenvpls(X, Y, m)
u =
   1
    ModelOutput = xenvpls(X, Y, u)
ModelOutput =
     beta: [3x1 double]
     SigX: [3x3 double]
    Gamma: [3x1 double]
    Gamma0: [3x2 double]
      eta: 5.2899
    Omega: 10.9286
    Omega0: [2x2 double]
       mu: 1.5683
    sigYcX: 1.0934
  paramNum: 9
       n: 64
```

ModelOutput.beta

```
ans = 0.2573 0.2741 0.3049
```

auxiliary

11.1 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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11.2 **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).

11.3 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).

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11.4 fit OLS

Fit 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 β.
- 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.asySE: The asymptotic standard error for elements in β . An r by p matrix. The standard errors returned are asymptotic, for actual standard errors, multiply by 1/sqrt(n).
- 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 ε contains the errors. This function performs the ordinary least squares fit to the inputs, and returns the estimates of β and the covariance matrix of ε .

Example

```
\label{eq:continuous_section} \begin{split} & load\ wheatprotein.txt \\ & X = wheatprotein(:, 8); \\ & Y = wheatprotein(:, 1:6); \\ & ModelOutput = fit\_OLS(X, Y) \\ & ModelOutput.betaOLS \end{split}
```

${\bf Model Output. Sigma OLS}$

```
{\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

11.5 get_envelope

Construct the envelope subspace using a sequential algorithm.

Contents

- Syntax
- Input
- Output
- Description
- Reference

Syntax

```
W = get envelope(S, M, u)
```

Input

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

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

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

Output

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

Description

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

Reference

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

Example

```
S = [1\ 2\ 3]';

S0 = grams(nulbasis(S'));

M = S * S' + S0 * S0';

u = 1;

W = get\_envelope(S, M, u)

W =
0.2673
0.5345
0.8018
```

11.6 get_Init

Generate starting value for the envelope subspace.

Contents

- Syntax
- Input
- Output
- Description
- Reference

Syntax

```
WInit = get Init(F, u, DataParameter)
```

Input

F: Objective function of the envelope subspace.

 ${f u}$: 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 the second one, then we record the vector. This goes on and on until the last one. We do it for 5 rounds and use the final set as our starting value.

Reference

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

11.7 get_Init4envmean

Generate starting value for the envelope subspace in estimating the multivariate mean.

Contents

- Syntax
- Input
- Output
- Description
- Reference

Syntax

```
WInit = get Init4envmean(F, u, DataParameter)
```

Input

F: Objective function to get the envelope subspace.

u: Dimension of the envelope. An integer between 1 and p - 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. A p by u orthogonal matrix.

Description

We compute the eigenvectors for the estimated error covariance matrix, and get p vectors. Then we get all the combinations of u vectors out of the p vectors. If the number of p 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 the second one, then we record the vector. This goes on and on until the last one. We do it for 3 rounds and use the final set as our starting value.

Reference

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

11.8 get_Init4henv

Generate starting value for the heteroscedastic envelope subspace.

Contents

- Syntax
- Input
- Output
- Description
- Reference

Syntax

```
WInit = get Init4henv(F, u, DataParameter)
```

Input

F: Objective function to get the heteroscedastic envelope subspace.

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 error covariance matrix, 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 the second one, then we record the vector. This goes on and on until the last one. We do it for 3 rounds and use the final set as our starting value.

Reference

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

11.9. KPD

11.9 Kpd

Compute the communication matrix Kpd.

Contents

- Syntax
- Input
- Output
- Description
- Reference

Syntax

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

Input

p, **d**: two positive integers represent the dimension parameters for the communication matrix.

Output

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

Description

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

Reference

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

11.10 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.

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11.11 make_dF

Generic function to generate the derivative function of the objective function E

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.

11.12 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.

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11.13 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 parameters 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 to print out output, logical 0 or 1.

Output:

Opts: A list containing optional input parameters 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 to 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.

11.14 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', '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 methods except 'henv'.
- DataParameter.invsigY: The inverse of the sample covariance matrix of Y. An r by r matrix. For all methods except 'ienv'.
- DataParameter.invsigRes: The inverse of the sample covariance matrix of the residuals form the ordinary least squares regression of Y on X. An r by r matrix. Only for method 'ienv'.

Description

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

11.15 mtest

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

Contents

- Syntax
- Input
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- References
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Syntax

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

Input

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

Y: Multivariate responses. An n by r matrix, r is the number of responses and n is number of observations. The responses must be continuous variables.

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

Output

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

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

Description

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

11.15. MTEST

References

The codes are implemented based on

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

Example

```
\begin{split} & load\ waterstrider.mat \\ & alpha = 0.01; \\ & TestOutput = mtest(X,\,Y,\,alpha); \end{split}
```

MBox	Chi-sqr.	df	Р			
157.5977	137.3361	72	0.0000			

Covariance matrices are significantly different.