

MATLAB Toolbox **envlp**: Reference Manual

February 17, 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.

Contents	2
1 tools	2
1.1 bootstrapse	2
1.2 bootstrapse_OLS	5
1.3 mfoldcv	7
1.4 modelselectaic	9
1.5 modelselectbic	11
1.6 modelselectlrt	13
1.7 prediction	15
1.8 testcoefficient	18
2 env	20
2.1 aic_env	20
2.2 bic_env	22
2.3 bstrp_env	24
2.4 dF4env	26
2.5 env	27
2.6 F4env	31
2.7 lrt_env	32
2.8 mfoldcv_env	34
2.9 predict_env	36
2.10 predict2_env	39
2.11 testcoefficient_env	42
3 envmean	44
3.1 aic_envmean	44
3.2 bic_envmean	46
3.3 bstrp_envmean	47
3.4 dF4envmean	49
3.5 envmean	50
3.6 F4envmean	53
3.7 lrt_envmean	54
3.8 mfoldcv_meanenv	56
3.9 predict_envmean	58
3.10 testcoefficient_envmean	60
4 envseq	62
4.1 bstrp_envseq	62
4.2 envseq	64
4.3 mfoldcv_envseq	66
5 henv	68
5.1 aic_henv	68
5.2 bic_henv	70
5.3 bstrp_henv	72
5.4 dF4henv	74
5.5 F4henv	75
5.6 henv	76
5.7 lrt_henv	79
5.8 mfoldcv_henv	81
5.9 predict_henv	83

5.10	testcoefficient_henv	86
6	ienv	88
6.1	aic_ienv	88
6.2	bic_ienv	90
6.3	bstrp_ienv	91
6.4	dF4ienv	93
6.5	F4ienv	94
6.6	ienv	95
6.7	lrt_ienv	98
6.8	mfoldcv_ienv	100
6.9	predict_ienv	102
6.10	testcoefficient_ienv	104
7	penv	106
7.1	aic_penv	106
7.2	bic_penv	108
7.3	bstrp_penv	110
7.4	lrt_penv	112
7.5	mfoldcv_penv	114
7.6	penv	116
7.7	predict_penv	119
7.8	testcoefficient_penv	122
8	senv	124
8.1	aic_senv	124
8.2	bic_senv	126
8.3	bstrp_senv	128
8.4	dF4senv	130
8.5	F4senv	131
8.6	mfoldcv_senv	132
8.7	objfun	134
8.8	predict_senv	135
8.9	senv	137
8.10	testcoefficient_senv	141
9	xenv	143
9.1	aic_xenv	143
9.2	bic_xenv	145
9.3	bstrp_xenv	147
9.4	dF4xenv	149
9.5	F4xenv	150
9.6	lrt_xenv	151
9.7	mfoldcv_xenv	153
9.8	predict_xenv	155
9.9	testcoefficient_xenv	157
9.10	xenv	159
10	xenvpls	163
10.1	bstrp_xenvpls	163
10.2	mfoldcv_xenvpls	165
10.3	xenvpls	167

11 auxiliary	169
11.1 center	169
11.2 Contr	170
11.3 Expan	171
11.4 fit_OLS	172
11.5 get_envelope	174
11.6 get_Init	175
11.7 get_Init4envmean	176
11.8 get_Init4henv	177
11.9 Kpd	178
11.10 Lmatrix	179
11.11 make_dF	180
11.12 make_F	181
11.13 make_opts	182
11.14 make_parameter	183
11.15 mtest	185

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.

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', 'penv', '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 for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

`bootse`: For `'env'`, `'envpls'`, `'henv'`, `'ienv'`, and `'senv'`, an r by p matrix containing the standard errors for elements in β computed by bootstrap. For `'penv'`, an r by p_1 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.

Example

```
load wheatprotein.txt
X = 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)
```

```
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 for 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.

Example

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

```
bootse =
```

```
10.2168
```


8.3940
9.0503
9.9677
14.5822
5.5874

1.3 mfoldcv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

This function implements m-fold cross validation to select the dimension of the envelope space, based on prediction performance. For each u , the data is partitioned into m parts, each part is in turn used for testing for the prediction performance while the rest $m-1$ parts are used for training. The dimension is 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(:, 8);
Y = wheatprotein(:, 1 : 6);
m = 5;
modelType = 'envpls';
u = mfoldcv(X, Y, m, modelType)
```

u =

0

1.4 modelselectaic

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

For model type '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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

This function implements the Akaike information criteria (AIC) to select the dimension of the envelope subspace for method 'env', 'henv', 'ienv', 'penv', 'senv', and 'xenv'.

Example

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1 : 6);
modelType = 'env';
u = modelselectaic(X, Y, modelType)
```

u =

1

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

This function implements the Bayesian information criteria (BIC) to select the dimension of the envelope subspace for method 'env', 'henv', 'ienv', 'penv', 'senv', and 'xenv'.

Example

```
load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1 : 6);
modelType = 'env';
u = modelselectbic(X, Y, modelType)
```

u =

1

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

This function implements the likelihood ratio testing procedure to select the dimension of the envelope subspace for method 'env', 'henv', 'ienv', 'penv', and 'xenv'. The likelihood ratio testing procedure does not support 'senv', because the scaled envelope models are not nested with the standard model.

Example

```
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

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

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

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

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

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

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

modelType: A string 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 $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. The covariance matrix and the standard errors are also provided.

Example

```

load wheatprotein.txt
X = wheatprotein(:, 8);
Y = wheatprotein(:, 1 : 6);
modelType = 'env';
u = modelselectbic(X, Y, modelType);
ModelOutput = env(X, Y, u);
Xnew = X(2, :);
PredictOutput = 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);
Xnew.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 $L * \beta * R \neq A$, where β 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', 'seenv' 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R - A) \hat{\Sigma}^{-1} \text{vec}(L\beta R - A)^T$, and the reference distribution is chi-squared distribution with degrees of freedom the same as the length of $\text{vec}(A)$.

Example

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

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

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
X.X1 = fiberpaper(:, 7);
X.X2 = fiberpaper(:, 5 : 6);
alpha = 0.01;
u = modelselectlrt(X, Y, alpha, 'penv');
ModelOutput = penv(X, Y, u);
r = size(Y, 2);
p1 = size(X.X1, 2);
TestInput.L = rand(2, r);
TestInput.R = rand(p1, 1);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_penv(ModelOutput, TestInput);
```

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

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

1

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

1

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 for 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.

Example

```
load wheatprotein.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
```

2.4 dF4env

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

$$\text{df} = \text{dF4env}(\mathbf{R}, \text{DataParameter})$$

Input

R: An r by u semi orthogonal matrix, $0 < u \leq r$.

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 \mathbf{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 for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- `Opts.init`: The initial value for the envelope subspace. An r by u matrix. Default value is the one generated by function `get_Init`.

Output

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

- `ModelOutput.beta`: The envelope estimator of the regression coefficients 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 semi-orthogonal 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 $r \times u$ by $r \times u$ 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 $\text{vec}(\beta)$. 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).

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

u =

1

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

```
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

```

```
ModelOutput.Omega
```

```
ans =
```

```
7.8762
```

```
eig(ModelOutput.Omega0)
```

```
ans =
```

```
1.0e+03 *
```

```

6.5166
0.2083
0.0201
0.0004
0.0003

```

```
ModelOutput.ratio
```

```
ans =
```

```
28.0389
```


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

$$f = \text{F4env}(R, \text{DataParameter})$$

Input

R: An r by u semi orthogonal matrix, $0 < u \leq r$.

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

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

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

Opts: A list containing the optional input 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

1

2.8 mfoldcv_env

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = mfoldcv_env(X, Y, m)
u = 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

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);
u = mfoldcv_env(X, Y, 5)
```

u =

1

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 indicating 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 $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. The covariance matrix and the standard errors are also provided.

Example

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

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

```
PredictOutput =
```

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

```
ans =
```

```
474.7135 468.0000
127.4740 123.0000
251.2044 246.0000
380.8280 374.0000
380.9473 386.0000
-6.3287 -11.0000
```

```
ans =
```

```
4.8892
4.0227
4.3237
4.7470
6.8186
2.6948
```

```
PredictOutput = predict_env(ModelOutput, Xnew, 'prediction')
PredictOutput.SE
```

```
PredictOutput =
```

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

```
ans =
```

```
474.7135
127.4740
251.2044
380.8280
380.9473
-6.3287
```



```
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 X_{new} . 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 X_{new} . It can perform estimation: find the fitted value when $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. 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.

Example

```

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
```

2.11 testcoefficient_env

This function tests the null hypothesis $L * \beta * R = A$ versus the alternative hypothesis $L * \beta * R \neq A$, where β 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_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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R - A) \hat{\Sigma}^{-1} \text{vec}(L\beta R - A)^T$, and the reference distribution is chi-squared distribution with degrees of freedom d1 * d2.

Example

```

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

```

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

```

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

```

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

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 for 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.

Example

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

```
u =
```

```
3
```

```
B = 100;
```

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

```
bootse =
```

```
0.5155
```

```
13.4169
```

```
13.2268
```

```
17.0221
```

```
21.4016
```

```
22.0329
```

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, $0 < u \leq p$.

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 for 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 semi-orthogonal 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 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.

- `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]
        l: -1.3492e+03
 covMatrix: [6x6 double]
```

```

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

```

ModelOutput.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

```

3.6 F4envmean

Objective function for computing the envelope subspace.

Contents

- Syntax
- Input
- Output
- Description

Syntax

$f = \text{F4envmean}(R, \text{DataParameter})$

Input

R: A p by u semi orthogonal matrix, $0 < u \leq p$.

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

2

3.8 mfoldcv_meanenv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = mfoldcv_meanenv(Y, m)
u = mfoldcv_meanenv(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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

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 Adopted
Y = Adopted(:, 1 : 6);
u = mfoldcv_envmean(Y, 5)
```

u =

1

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.

Example

```
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]
```

```
PredictOutput.value
```

```
ans =
```

```
12.3258  
85.9841  
115.5767  
112.1291  
114.4862  
106.4240
```

```
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 $L * \mu \neq A$, where μ 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 $L\mu$. 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.

Example

```

load Adopted
Y = Adopted(:, 1 : 6);
u = bic_envmean(Y);
ModelOutput = envmean(Y, u);
TestOutout = testcoefficient_envmean(ModelOutput);

```

Test Hypothesis	Chisq Statistic	DF	P-value
L * mu = A	8716.691	6	0.0000

```

p = size(Y, 2);
TestInput.L = rand(2, p);
TestInput.A = zeros(2, 1);
TestOutout = testcoefficient_envmean(ModelOutput, TestInput);

```

Test Hypothesis	Chisq Statistic	DF	P-value
L * mu = A	6543.508	2	0.0000

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 for 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.

Example

```
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
```

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 semi-orthogonal 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

```
u = mfoldcv_envseq(X, Y, m)
u = 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

This function implements m-fold cross validation to select the dimension of the envelope space, based on prediction performance. For each u, the data is partitioned into m parts, each part is in turn used for testing for the prediction performance while the rest m-1 parts are used for training. The dimension is 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 Rohwer
X = Rohwer(:, 4 : 5);
Y = Rohwer(:, 1 : 3);
m = 5;
```

```
u = mfoldcv_envpls(X, Y, m)
```

```
u =
```

```
1
```

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

6

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

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 for 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.

Example

```
load waterstrider.mat

u = lrt_henv(X, Y, 0.01)

u =

    6

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

bootse =

    0.0305    0.0466    0.0647
    0.0309    0.0485    0.0682
    0.0305    0.0432    0.0638
    0.0205    0.0289    0.0425
    0.0385    0.0553    0.0799
    0.0295    0.0427    0.0618
    0.0389    0.0567    0.0819
    0.0321    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, $0 < u \leq r$.

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.

5.5 F4henv

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

$f = \text{F4henv}(R, \text{DataParameter})$

Input

R: An r by u semi orthogonal matrix, $0 < u \leq r$.

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

Output

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

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

- `ModelOutput.Gamma`: The orthogonal basis of the envelope subspace. An r by u semi-orthogonal 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 i th column of the matrix contains the main effect for the i th group.
- `ModelOutput.groupInd`: A matrix containing the unique values of group indicators. The matrix has p rows. The group mean of the i th row is stored in the i th 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 i th group.
- `ModelOutput.eta`: The coordinates of β with respect to `Gamma`. A u by p matrix, the i th column contains the coordinates of the main effect of the i th 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 i th 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 $1 / \text{sqrt}(n)$.
- `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 i th element in the j th 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 Lipert (<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 5.0351 4.6347
4.1925 4.7967 4.2595
4.5553 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

```

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

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

Input

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

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

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

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

```
u = mfoldcv_henv(X, Y, m)
u = mfoldcv_Henv(X, Y, m, 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.

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

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

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

Output

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

Description

This function implements 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 waterstrider.mat  
u = mfoldcv_henv(X, Y, 5)
```

u =

2

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 indicators from the original data.

infType: A string of characters indicating 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.

Example

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

```
ans =
```

```
-1  -1
 0   1
 1   0
```

```
ans =
```

```
-1.1417 -1.1267 -1.0845
-1.4063 -1.4067 -1.3132
-1.3314 -1.3336 -1.2152
-0.3113 -0.1839 -0.1736
 0.4003  0.3847  0.3072
 0.4107  0.3753  0.3735
 0.3467  0.3271  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
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')  
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 $L * \beta * R \neq A$, where β 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R)$. A d1 * d2 by d1 * d2 matrix.

Description

This function tests for hypothesis $H_0 : L\beta R = A$, versus $H_a : L\beta R \neq A$. 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 $\text{vec}(L\beta R - A) \hat{\Sigma}^{-1} \text{vec}(L\beta R - A)^T$, and the reference distribution is chi-squared distribution with degrees of freedom d1 * d2.

Example

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

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

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

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

ienv

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

1

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

1

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 or equal to 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 for 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.

Example

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

u =

1

B = 100;

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

bootse =

13.4695	4.9601
7.4709	2.7315
14.9316	5.2913
8.7597	3.0853

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, $0 < u \leq p$.

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

$$f = \text{F4ienv}(R, \text{DataParameter})$$

Input

R: An r by u semi orthogonal matrix, $0 < u \leq p$.

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.

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

Output

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

- `ModelOutput.beta`: The envelope estimator of the regression coefficients 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 Γ_1 . A p by u matrix.
- `ModelOutput.B`: An $(r - u)$ by $(p - u)$ semi-orthogonal matrix, so that $(\Gamma_1, \Gamma_0 * B)$ spans β .
- `ModelOutput.eta2`: The transpose of the coordinates of β with respect to Γ_0 . A p by $(p - u)$ matrix.
- `ModelOutput.Omega1`: The coordinates of Σ with respect to Γ_1 . A u by u matrix.
- `ModelOutput.Omega0`: The coordinates of Σ with respect to Γ_0 . 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 $\text{vec}(\beta)$. 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 Lipert (<http://web.mit.edu/~ripper/www/sgmin.html>).

Example

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

```
load irisf.mat

d = bic_ienv(X, Y)
```

d =

```
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+03
    covMatrix: [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

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

Input

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

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

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

Opts: A list containing the optional input 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

```
load irisf.mat

alpha = 0.01;
u = lrt_ienv(X, Y, alpha)
```

u =

1

6.8 mfoldcv_ienv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = mfoldcv_ienv(X, Y, m)
u = 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

u: The dimension of the inner envelope subspace selected by m-fold cross validation. An integer between 0 and p or equal to r.

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
u = mfoldcv_ienv(X, Y, 5)
```

$$u =$$

$$0$$

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 indicating 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 $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. The covariance matrix and the standard errors are also provided.

Example

```
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
```

```
PredictOutput =
```

```
    value: [4x1 double]
  covMatrix: [4x4 double]
      SE: [4x1 double]
```

```
ans =
```

```
49.9458  51.0000
34.2592  35.0000
14.5771  14.0000
 2.4513   2.0000
```

```
ans =
```

```
1.0978
0.7146
0.9265
0.4357
```

```
PredictOutput = predict_ienv(ModelOutput, Xnew, 'prediction')
PredictOutput.SE
```

```
PredictOutput =
```

```
    value: [4x1 double]
  covMatrix: [4x4 double]
      SE: [4x1 double]
```

```
ans =
```

```
5.2197
3.3897
4.3996
2.0642
```

6.10 testcoefficient_ienv

This function tests the null hypothesis $L * \beta * R = A$ versus the alternative hypothesis $L * \beta * R \neq A$, where β 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R - A) \hat{\Sigma}^{-1} \text{vec}(L\beta R - A)^T$, and the reference distribution is chi-squared distribution with degrees of freedom d1 * d2.

Example

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

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

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

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

7.1 aic_penv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

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

Opts: A list containing the optional input 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
X.X1 = fiberpaper(:, 7);
X.X2 = fiberpaper(:, 5 : 6);
u = aic_penv(X, Y)
```

u =

3

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

```
load fiberpaper.dat
Y = fiberpaper(:, 1 : 4);
X.X1 = fiberpaper(:, 7);
X.X2 = fiberpaper(:, 5 : 6);
u = bic_penv(X, Y)
```

u =

1

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 for 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.

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')

u =

    1

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

bootse =

    0.0074
    0.0021
    0.0043
    0.0019
```

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

1

7.5 mfoldcv_penv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = mfoldcv_penv(X, Y, m)
u = mfoldcv_penv(X, Y, m, 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.

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

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

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

Output

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

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 = fiberpaper(:, 1 : 4);
X.X1 = fiberpaper(:, 7);
X.X2 = fiberpaper(:, 5 : 6);
u = mfoldcv_penv(X, Y, 5)
```

u =

0

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 p_1 matrix, n is the number of observations, and p_1 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 p_2 matrix, p_2 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 for print out Grassmann manifold optimization process, logical 0 or 1. Default value: 0.
- **Opts.init:** The initial value for the partial envelope subspace. An r by u matrix. Default value is the one generated by function `get_Init`.

Output

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

- **ModelOutput.beta1:** The partial envelope estimator of β_1 , which is the regression coefficients for X1. An r by p_1 matrix.
- **ModelOutput.beta2:** The partial envelope estimator of β_2 , which is the regression coefficients for X2. An r by p_2 matrix.

- `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 p_1 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 r_p by r_p 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 p_1 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 p_1 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 X_1 and X_2 , 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 X_1 and X_2 as predictors. When the dimension is 0, X_1 and Y are uncorrelated, and the fitting is the standard multivariate linear regression with Y as the responses and X_2 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)
ModelOutput.Omega
eig(ModelOutput.Omega0)
ModelOutput.ratio
```

```
ModelOutput =
```

```
beta1: [4x1 double]
beta2: [4x2 double]
alpha: [4x1 double]
Gamma: [4x1 double]
eta: 0.0047
Omega: 0.0149
Omega0: [3x3 double]
Sigma: [4x4 double]
l: -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 $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. The covariance matrix and the standard errors are also provided.

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);
Xnew.X1 = X.X1(1, :);
Xnew.X2 = X.X2(1, :);
PredictOutput = predict_penv(ModelOutput, Xnew, 'estimation')
[PredictOutput.value, Y(1, :)] % Compare the fitted value with the data
PredictOutput.SE

```

```
PredictOutput =
```

```

    value: [4x1 double]
covMatrix: [4x4 double]
      SE: [4x1 double]

```

```
ans =
```

```

21.1169  21.3120
 7.1173   7.0390
 5.3637   5.3260
 0.8737   0.9320

```

```
ans =
```

```

1.4680
0.4234
0.7145
0.3161

```

```

PredictOutput = predict_penv(ModelOutput, Xnew, 'prediction')
PredictOutput.SE

```

```
PredictOutput =
```

```

    value: [4x1 double]
covMatrix: [4x4 double]
      SE: [4x1 double]

```

```
ans =
```

```

2.4277

```

0.6982

1.1802

0.5220

7.8 testcoefficient_penv

This function tests the null hypothesis $L * \beta_1 * R = A$ versus the alternative hypothesis $L * \beta_1 * R \neq A$, where β_1 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 d_1 by r matrix, while d_1 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 p_1 by d_2 matrix, while d_2 is less than or equal to p_1 . Default value: identity matrix I_{p_1} .
- **TestInput.A:** The matrix on the right hand side of the equation. It is a d_1 by d_2 matrix. Default value: d_1 by d_2 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 $\text{vec}(L\beta_1 R)$. 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 $\text{vec}(L\beta_1 R)$. A $d_1 * d_2$ by $d_1 * d_2$ matrix.

Description

This function tests for hypothesis $H_0 : L\beta_1 R = A$, versus $H_a : L\beta_1 R \neq A$. 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 $\text{vec}(L\beta_1 R - A)^T \hat{\Sigma}^{-1} \text{vec}(L\beta_1 R - A)$, and the reference distribution is chi-squared distribution with degrees of freedom $d_1 * d_2$.

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

8.1 aic_senv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

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

Input

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

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

Opts: A list containing the optional input 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 for print out dimension selection process, 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 Akaike information criteria (AIC) to select the dimension of the scaled envelope subspace.

Example

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

u =

4

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 for print out dimension selection process, 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.

Example

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

u =

2

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.

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 for 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.

Example

```
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	0.0554
0.0675	0.0912	0.1178
0.0567	0.0781	0.0791
0.0986	0.0944	0.1283

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, $0 < u \leq r$.

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.

8.5 F4senv

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

$f = \text{F4senv}(R, \text{DataParameter})$

Input

R: An r by u semi orthogonal matrix, $0 < u \leq r$.

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.

8.6 mfoldcv_senv

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

Contents

- Syntax
- Input
- Output
- Description
- Example

Syntax

```
u = mfoldcv_senv(X, Y, m)
u = 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 for print out dimension selection process, 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: The dimension of the scaled envelope subspace selected by m-fold cross validation. An integer between 0 and r.

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

```
load('sales.txt')
Y = sales(:, 4 : 7);
X = sales(:, 1 : 3);
u = mfoldcv_senv(X, Y, 5)
```

u =

2

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 r th 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 from 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.

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 indicating 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 X_{new} . 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 X_{new} . It can perform estimation: find the fitted value when $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. The covariance matrix and the standard errors are also provided.

Example

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

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

```
PredictOutput =
```

```
value: [4x1 double]
covMatrix: [4x4 double]
SE: [4x1 double]
```

```
ans =
```

```
8.9109    9.0000
11.5096   12.0000
9.6063    9.0000
19.5119   20.0000
```

```
ans =
```

```
7.7627
5.8952
4.2205
8.0134
```

```
PredictOutput = predict_senv(ModelOutput, Xnew, 'prediction')
PredictOutput.SE
```

```
PredictOutput =
```

```
value: [4x1 double]
covMatrix: [4x4 double]
SE: [4x1 double]
```

```
ans =
```

```
8.3024
6.3052
4.4254
8.5956
```

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 for 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.

- `ModelOutput.Gamma`: The orthogonal basis of the envelope subspace. An r by u semi-orthogonal 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 Σ with respect to `Gamma`. A u by u matrix.
- `ModelOutput.Omega0`: The coordinates of Σ 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 $\text{vec}(\beta)$. 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 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 X and Y 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).

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

`u =`

```
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
```

```
ModelOutput.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.

```
load('Urine.txt')
Y = Urine(:, 3 : 11);
X = Urine(:, 12 : 14);
Opts.rep = [6 3];
u = bic_senv(X, Y, Opts)
```

```
u =
```

```
1
```

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

```
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
```

8.10 testcoefficient_senv

This function tests the null hypothesis $L * \beta * R = A$ versus the alternative hypothesis $L * \beta * R \neq A$, where β 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R - A)^T \hat{\Sigma}^{-1} \text{vec}(L\beta R - A)$, and the reference distribution is chi-squared distribution with degrees of freedom $d1 * d2$.

Example

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

Test Hypothesis	Chisq Statistic	DF	P-value
L * beta * R = A	4660.161	12	0.0000

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

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

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

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The 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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

4

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

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 for 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.

Example

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

u =

4

```
B = 100;
bootse = bstrp_xenv(X, Y, u, B)
```

bootse =

```
0.0385
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, $0 < u \leq p$.

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

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

$f = \text{F4xenv}(R, \text{DataParameter})$

Input

R: A p by u semi orthogonal matrix, $0 < u \leq p$.

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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

Description

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

Example

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

u =

4

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

```
u = mfoldcv_xenv(X, Y, m)
u = mfoldcv_xenv(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 for print out dimension selection process, logical 0 or 1. Default value: 0.

Output

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

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);
u = mfoldcv_xenv(X, Y, 5)
```

u =

4

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 $X = X_{\text{new}}$, or prediction: predict Y when $X = X_{\text{new}}$. The covariance matrix and the standard errors are also provided.

Example

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

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

PredictOutput =

    value: 9.1751
covMatrix: 16.8439
    SE: 4.1041

ans =

    9.1751    9.2300

ans =

    4.1041

PredictOutput = predict_xenv(ModelOutput, Xnew, 'prediction')
PredictOutput.SE

PredictOutput =

    value: 9.1751
covMatrix: 16.8760
    SE: 4.1080

ans =

    4.1080
```

9.9 testcoefficient_xenv

This function tests the null hypothesis $L * \beta * R = A$ versus the alternative hypothesis $L * \beta * R \neq A$, where β 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 $\text{vec}(L\beta R)$. 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 $\text{vec}(L\beta R)$. A $d1 * d2$ by $d1 * d2$ matrix.

Description

This function tests for hypothesis $H_0 : L\beta R = A$, versus $H_a : L\beta R \neq A$. 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 $\text{vec}(L\beta R - A) \hat{\Sigma}^{-1} \text{vec}(L\beta R - A)^T$, and the reference distribution is chi-squared distribution with degrees of freedom $d1 * d2$.

Example

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

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

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

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

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 for 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 semi-orthogonal 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 $\text{vec}(\beta)$. 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 Lipert (<http://web.mit.edu/~ripper/www/sgmin.html>).

Example

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

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

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

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

```
ans =
```

```
0.0321
```

```
ans =
```

```
0.0321
```

```
temp.betaOLS'
ModelOutput.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)
```

```
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 for 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.

Example

```
load VocabGrowth
X = VocabGrowth(:, 1 : 3);
Y = VocabGrowth(:, 4);
m = 5;
u = mfoldcv_xenvpls(X, Y, m)
```

u =

1

```
B = 100;
bootse = bstrp_xenvpls(X, Y, u, B)
```

bootse =

```
0.0230
0.0235
0.0273
```

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

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

Input

X: Predictors. An n by p matrix, p is the number of predictors and n is number of observations. The 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 for print out the number of bootstrap samples, logical 0 or 1. Default value: 0.

Output

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

Description

This function implements m-fold cross validation to select the dimension of the envelope space, based on prediction performance. For each u, the data is partitioned into m parts, each part is in turn used for testing for the prediction performance while the rest m-1 parts are used for training. The dimension is 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 VocabGrowth
X = VocabGrowth(:, 1 : 3);
Y = VocabGrowth(:, 4);
m = 5;
u = mfoldcv_xenvpls(X, Y, m)
```


u =

1

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 semi-orthogonal 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.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, 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
```

11.1 center

Subtract the mean of each column.

Contents

- Syntax
- Input
- Output
- Description

Syntax

$$XC = \text{center}(X)$$

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.

11.2 Contr

Compute the contraction matrix of dimension r .

Contents

- Syntax
- Input
- Output
- Description

Syntax

$$C = \text{Contr}(r)$$

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 , $\text{vech}(A) = \text{Contr}(r) * \text{vec}(A)$, and $\text{vec}(A) = \text{Expan}(r) * \text{vech}(A)$. 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).

11.3 Expan

Compute the expansion matrix of dimension r .

Contents

- Syntax
- Input
- Output
- Description

Syntax

$E = \text{Expan}(r)$

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 , $\text{vech}(A) = \text{Contr}(r) * \text{vec}(A)$, and $\text{vec}(A) = \text{Expan}(r) * \text{vech}(A)$. 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).

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

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

ModelOutput.SigmaOLS

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

$$W = \text{get_envelope}(S, M, u)$$

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 $\text{span}(S)$.

Description

This function constructs the M -envelope of $\text{span}(S)$ 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

$$W_{\text{Init}} = \text{get_Init}(F, u, \text{DataParameter})$$

Input

F: Objective function of the 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 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

Compute the communication matrix Kpd.

Contents

- Syntax
- Input
- Output
- Description
- Reference

Syntax

$$k = \text{Kpd}(p, d)$$

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 , $\text{vec}(A') = \text{Kpd} * \text{vec}(A)$, 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

$$L = \text{Lmatrix}(r)$$

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 $\text{Lmatrix}(r) * \text{vec}(A)$ will give the 2nd to the r th diagonal elements of A , arranged in a column vector.

11.11 make_dF

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

Contents

- Syntax
- Input
- Output
- Description

Syntax

```
dF = make_dF(dfun_method_handle, FParameters)
```

Input

- `dfun_method_handle`: A specific model derivative function of the objective function.
- `FParameters`: A structure that contains data parameters as input for the function `dfun_method_handle`.

Output

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

Description

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

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.

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 for 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 for print out output, logical 0 or 1. Default value: 0.

Description

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

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', 'henv', 'senv' or 'xenv'.

Output

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

- **DataParameter.n:** The number of observations in the data. A positive integer.
- **DataParameter.ng:** A p by 1 vector containing the number of observations in each group. p is the number of groups. Only for 'henv'.
- **DataParameter.ncum:** A p by 1 vector containing the total number of observations till this group. Only for 'henv'.
- **DataParameter.ind:** An n by 1 vector indicating the sequence of the observations after sorted by groups.
- **DataParameter.p:** The number of predictors or number of groups for 'henv'. A positive integer.
- **DataParameter.r:** The number of responses. A positive integer.
- **DataParameter.XC:** Centered predictors. An n by p matrix with the i th row being the i th 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 i th row being the i th 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 i th column being the sample mean of the i th 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 from 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
- Output
- Description
- References
- Example

Syntax

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

Input

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

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

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 homogeneity 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.

References

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

Example

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

MBox	Chi-sqr.	df	P
157.5977	137.3361	72	0.0000

Covariance matrices are significantly different.