Statistical Learning based Estimation of the Mutual Information (SLEMI) - R package

User Manual

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Abstract

The SLEMI package is designed to estimate channel capacity, mutual information, and probabilities of correct discrimination for signaling systems with a discrete input and multidimensional continuous output. SLEMI is released under the GNU license and is freely available from GitHub. Comprehensive documentation is available also on github.io. In case of any bugs, problems, or other questions contact t.jetka at sysbiosig.org and/or m.komorowski at sysbiosig.org. The package, is a part of the paper *Jetka et al., Information-theoretic analysis of multivariate signaling responses using SLEMI*. The above paper is hereafter referred to as *Main Paper* (**MP**). The Supplementary Information of the paper will be referred to as **SI**.

Contents

1 Preliminaries

1.1 Requirements - Hardware

- A 32 or 64 bit processor (recommended: 64bit)
- 1GHz processor (recommended: multicore for a comprehensive analysis)
- 2GB MB RAM (recommended: 4GB+, depends on the size of experimental data)

1.2 Requirements - Software

The main software requirement is the installation of the R environment (version: >= 3.2), which can be downloaded from R project website and is distributed for all common operating systems. We tested the package in R environment installed on Windows 7, 10; Mac OS X 10.11 - 10.13 and Ubuntu 18.04 with no significant differences in the performance. The use of a dedicated Integrated development environment (IDE), e.g. RStudio is recommended.

Apart from a base installation of R, SLEMI requires the following R packages:

1. for installation

- devtools

2. for estimation

- e1071
- Hmisc
- nnet
- glmnet
- caret
- doParallel (if parallel computation are needed)

3. for visualisation

- ggplot2
- ggthemes
- gridExtra
- corrplot

4. for data handling

- reshape2
- stringr
- plyr

Each of the above packages can be installed by executing

```
install_packages("name_of_a_package")
```

in the R console. During installation availability of the above packages will be verified and missing packages will be automatically installed.

1.3 Installation

The package can be directly installed from GitHub. For installation, open RStudio (or base R) and run following commands in the R console

```
install_packages("devtools") # run if 'devtools' is not installed
library(devtools)
install_github("sysbiosig/SLEMI")
```

Are required packages not found, they will be installed automatically.

2 Structure of the package

The three functions listed below constitute the key wrapper (interface) functions of the package.

1. `mi_logreg_main()` enables calculation of the mutual information
2. `capacity_logreg_main()` enables calculation of the information capacity
3. `prob_discr_pairwise()` serves to calculate probabilities of correct discrimination between pairs of input values

Below, we outline the architectures of these functions.

The function `capacity_logreg_main()` triggers

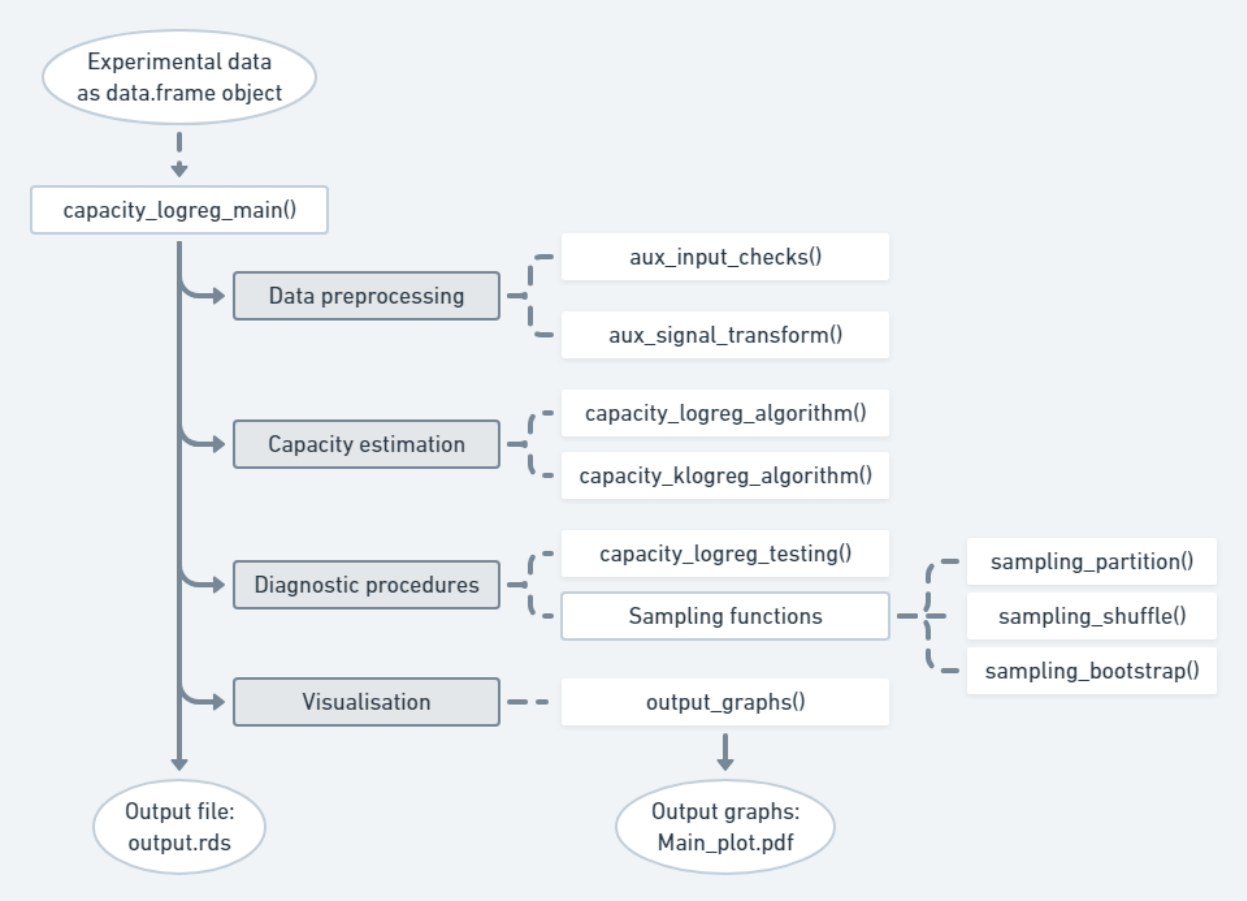
i) preprocessing of the data

ii) estimation of channel capacity

iii) running diagnostic procedures

iv) visualisation.

Each of the above steps is implemented in auxiliary functions as presented by the graph below.



The algorithm to compute the information capacity is implemented within the function `capacity_logreg_algorithm()`, which uses logistic regression from the `nnet package`.

Diagnostic procedures (significance and uncertainties of estimates) are provided in the function `capacity_logreg_testing()`. Those are based on data bootstrapping and overfitting test.

For visualization, a set of graphs is created by the function `capacity_output_graphs()` and saved in a specified directory.In addition, `capacity_logreg_main()` returns a list with capacity estimates, optimal input probability distribution, diagnostic measures and other summary information about the analysis.

The function `mi_logreg_main()` serves to calculate the mutual information. It initiates similar steps as the function `capacity_logreg_main()` but without performing the optimization of the distribution of the input. Instead, it expects that this distribution is given by the user.

Then, following an analogous algorithm as for channel capacity, logistic regression and Monte Carlo methods are combined to estimate mutual information within a function `mi_logreg_algorithm()`. Visualisation and diagnostics are carried out by the same set of auxillary functions as for channel capacity (`capacity_output_graphs()` and `capacity_logreg_testing()`).

The `prob_discr_pairwise()` is a standalone function that allows to estimate probabilities of discrimination between two different values of the input. It implements estimation of probabilities of correct classification by logistic regression (from `nnet` package) for each pair of input values. They are visualised by a graph of pie charts.

2.1 Input data

Functions `mi_logreg_main()`, `capacity_logreg_main()`, `prob_discr_pairwise()` require data in form of the object `data.frame` with a specifc structure of rows and columns. As described in detail in Section 1 of the **SI**, single cell responses y_j^i are assumed to be measured for a finite set of stimuli levels $x_1, x_2, \ldots, x_m$. The responses y_j^i can be multidimensional. Usually, experimental dataset is represented as a table with rows and columns organized as below

input	output 1	output 2	output 3	...
n_1 { x_1	$y_1^1(1)$	$y_1^1(2)$	$y_1^1(3)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	
x_1	$y_{n_1}^1(1)$	$y_{n_1}^1(2)$	$y_{n_1}^1(3)$	
n_2 { x_2	$y_1^2(1)$	$y_1^2(2)$	$y_1^2(3)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	
x_2	$y_{n_2}^2(1)$	$y_{n_2}^2(2)$	$y_{n_2}^2(3)$	
				...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	
n_m { x_m	$y_1^m(1)$	$y_1^m(2)$	$y_1^m(3)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	
x_m	$y_{n_m}^m(1)$	$y_{n_m}^m(2)$	$y_{n_m}^m(3)$	

Therefore, the input data frame is expected to have the form represed by the above table, which can be formally described by the following conditions

- each row represent a response of a single cell
- first column contains values of the input (X).
- second and subsequent columns contain values of the measured output(s); those columns should be of type `numeric`; order and number of outputs should be the same for all cells.
- the number of unique values of the input should be finite
- a large number of observations, possibly >100, per input value is required.

An example of the input `data.frame`, which contains the measurements of the NfkB system presented in the **MP** is available within the package under the variable `data_nfkb`. It has the following format

	signal	response_0	response_3	response_6
1	0ng	0.3840744	0.4252835	0.4271986
2	0ng	0.4709216	0.5777821	0.5361948
3	0ng	0.4274474	0.6696011	0.8544916
10001	8ng	0.3120216	0.3475484	1.0925967
10002	8ng	0.2544961	0.6611051	2.2894928
10003	8ng	0.1807391	0.4336810	1.9783171
11540	100ng	1.3534083	3.0158004	5.1592848
11541	100ng	1.7007936	2.2224497	3.5463418
11542	100ng	0.1997087	0.2886905	1.9324093

where each row represents measurements of a single-cell, the column named `signal` specifies the level of stimulation, while response_T is the response of the NfkB system in an individual cell at time point T. The above table can be shown in R by calling

```
library(SLEMI)
rbind(data_nkfb[1:3,1:4],data_nkfb[10001:10003,1:4],tail(data_nkfb[,1:4],3))
```

2.2 Calculation of the information capacity

Calculation of the information capacity with the default settings is perfomed by the command

```
capacity_logreg_main(dataRaw,signal, response, output_path)
```

where the required arguments are

- `dataRaw` - data frame with column of type `factor` containing values of input (X) and columns of type `numeric` containing values of output (Y), where each row represents a single observation
- `signal` - a character which indicates the name of the column in `dataRaw` with values of input (X)
- `response` - a character vector which indicates the names of columns in `dataRaw` with values of output (Y)
- `output_path` - a character with the directory, to which output should be saved

The function returns a list with the following elements

- cc - a numeric with channel capacity estimate (in bits)
- p_opt - a numeric vector with the optimal input distribution
- model - a `nnet` object describing fitted logistic regression model
- data - a data.frame with the raw experimental data (if `dataout=TRUE`)
- time - processing time of the algorithm
- params - a vector of parameters used in the algorithm
- regression - a confusion matrix of logistic regression predictions
- logGraphs - a list of gg or ggtables objects with a standard set of exploratory graphs

By default, all returned elements are saved in `output_path` directory in a file `output.rds`. Along with the output data, results of the computations are visualised as the graphs listed below

- MainPlot.pdf - a simple summary plot with basic distribution visualization and capacity estimate
- MainPlot_full.pdf - a comprehensive summary plot with distribution visualization and capacity estimate
- capacity.pdf - a diagram presenting the capacity estimates
- io_relation.pdf - a graph with input-output relation
- kdensities.pdf - kernel density estimator of data distribution
- histograms.pdf - histograms of data
- boxplots.pdf - boxplots of data
- violin.pdf - violin plots of data

2.3 Calculation of the mutual information

The function `mi_logreg_main()` takes a similar list of arguments and generates analogous plots to the function `capacity_logreg_main()`. The differences are listed below.

Firstly, user must specify the distribution of input that should be used in calculation of mutual information by passing a numeric vector via the argument `pinput` of `mi_logreg_main()` function. Secondly, the returned list stores the value of the computed mutual information (in bits) under the element `mi`, which is a numeric.

2.4 Calculation of the probabilities of correct discrimination

Calculation of the probabilities of correct discrimination between pairs of input values is performed by running the following command

```
prob_discr_pairwise(dataRaw,signal, response, output_path)
```

where the required arguments are analogous to arguments of the functions `capacity_logreg_main()` and `mi_logreg_main()`. The probabilities of correct discrimination are computed for each pair of unique input values and returned as a list with the following elements

- prob_matr - a symmetric numeric matrix with a probability of discriminating between i-th and j-th input values in cell (i,j)
- model - a list of `nnet` objects describing fitted logistic regression models of classification two chosen input values.

In addition, a plot of corresponding pie charts is created in `output_path` in the pdf format.

3 Diagnostic procedures

In addition to sole calculation of the information capacity, the function `capacity_logreg_main()` can also be used to asses accuracy of the channel capacity estimates resulting from finite sample size and over-fitting of the regression model. Two test are implemented. Precisely, the function can perfom

1. Bootstrap test - capacity is re-calculated using $\alpha\%$ of data, sampled from the original dataset without replacement. After repeating the procedure n times, its standard deviation can serve as an error of the obtained capacity estimate.
2. Over-fitting test - the original data is divided into Training and Testing datasets. Then, logistic regression is estimated using $\alpha\%$ of data (training dataset), and integrals of channel capacity are calculated via Monte Carlo using remaining $(1-\alpha)\%$ of data (testing dataset). It is repeated n times.

In order to perform diagostic tests, that by default are turned off, user must set the value of the input argument

- testing = TRUE (default=FALSE)

In addition, settings of the diagnostic test can be altered with the following paramaters

- TestingSeed (default= 1234) - the seed for the random number generator used to sample original dataset,
- testing_cores (default= 4) - a number of cores to use (via `doParallel` package) in parallel computing,
- boot_num (default= 40) - a number of repetitions of the bootstrap ,
- boot_prob (default= 0.8) - a fraction of initial observations to use in the bootstrap,
- traintest_num (default= 40) - a number of repetitions of the overfitting test,
- partition_trainfrac (default= 0.6) - a fraction of initial observations to use as a training dataset in the overfitting test

4 Additional functionalities of the function `capacity_logreg_main()`

In addition, to the basic functionalities described above, the function `capacity_logreg_main()` allows to control several other paramters of the alorithm that computes the information capacity. These parameters and their effects are listed below.

- `model_out` (`default=TRUE`) - logical, specify if `nnet` model object should be saved into output file
- `graphs` (`default=TRUE`) - logical, controls creating diagnostic plots in the output directory.
- `plot_width` (`default = 6`) - numeric, the basic width of created plots
- `plot_height` (`default = 4`) - numeric, the basic height of created plots
- `scale` (`default = TRUE`) - logical, value indicating if the columns of `dataRaw` are to be centered and scaled, what is usually recommended for the purpose of stability of numerical computations. From a purely theoretical perspective, such transformation does not influence the value of channel capacity.
- `lr_maxit` (`default = 1000`) - a maximum number of iterations of fitting step of logistic regression algorithm in `nnet` function. If a warning regarding lack of convergence of logistic model occurs, should be set to a larger value (possible if data is more complex or of a very high dimension).
- `MaxNWts` (`default = 5000`) - a maximum number of parameters in logistic regression model. A limit is set to prevent accidental over-loading the memory. It should be set to a larger value in case of exceptionally high dimension of the output data or very high number of input values. In principle, logistic model requires fitting $(m-1)\cdot(d+1)$ parameters, where m is the number of unique input values and d is the dimension of the output.

The latter two parameters, i.e `lr_maxit` and `MaxNWts`, allow to change the parameters of the logistic regression model fitting within the dependent `nnet` package.

5 Examples

5.1 Minimal example

Below, we present a minimal model that may serve as a quick introduction to computations within the package. Precisely, we consider a system

i) with four different input values X: 0, 0.1, 1 and 10
ii) with the conditional output, $Y|X = x$, give by a one-dimensional log-normal distribution $\exp\{\mathcal{N}(10 \cdot \frac{x}{1+x}, 1)\}$
iii) and the sample consisting of 1000 observations for each input value.

The example is analogous to the Test example 2 of the **SI** (Section 3.2).

Input data

Firstly, we generate a a synthetic dataset. The data corresponding to the model can be generated, and represented as the data frame `tempdata` with columns `input` and `output`, by running

```
xs=c(0,0.1,1,10) # concentration of input.
tempdata = data.frame(input = factor(c(t(replicate(1000,xs))),
                      levels=xs),
                      output =  c(matrix(rnorm(4000, mean=10*(xs/(1+xs)),sd=c(1,1,1,1)),
                                         ncol=4,byrow=TRUE) ))
```

The generated data.frame has the following structure

	input	output
1	0	0.5152491
2	0	1.0203139
2001	1	4.8705941
2002	1	6.0001276
3999	10	8.9778724
4000	10	9.5236630

Calculation of the information capacity

The Information capacit can be calculated using the `capacity_logreg_main()` function that takes the data frame "tempdata" as `dataRaw` argument. Column names "input" and "output" are used as arguments `signal` and `response`, respectively. The `output_path` is set as "minimal_example/". Therefore, the function is run as follows

```
tempoutput  <- capacity_logreg_main(dataRaw=tempdata,
                                    signal="input", response="output",
                                    output_path="minimal_example/")
```

Results of the computations are returned as a data structure described before. In addition, results are presented in the form of the following graph (by default saved as MainPlot.pdf in `minimal_example/` directory). It represents the input-output data and gives the corresponding channel capacity.

Calculation of the mutual information

To compare mutual information of experimental data with its channel capacity, we can run (uniform distribution of input values is assumed)

```
tempoutput_mi  <- mi_logreg_main(dataRaw=tempdata,
                                 signal="input", response="output",
```

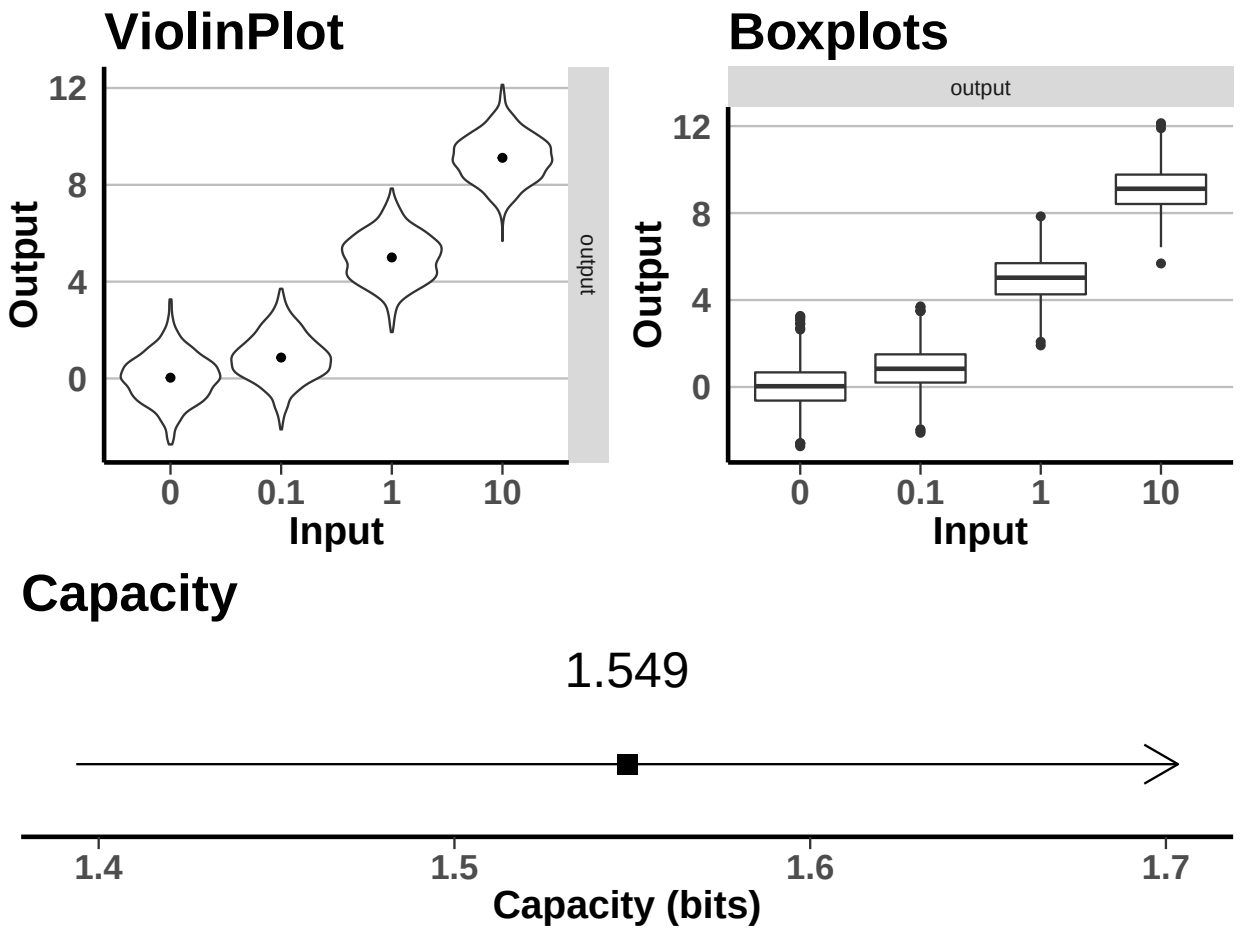


Figure 1: Standard output graph of the minimal working example

```
                                    output_path="minimal_exampleMI/",
                                    pinput=rep(1/4,4))
```

and display results

```
print(paste("Mutual Information:", tempoutput_mi$mi,"; ",
            "Channel Capacity:", tempoutput$cc, sep=" "))
```

```
## [1] "Mutual Information: 1.48864924701936 ;  Channel Capacity: 1.54854509707652"
```

Calculation of the probabilities of correct discrimination

Probabilities of correct discrimination between input values are calculated as follows

```
tempoutput_probs  <- prob_discr_pairwise(dataRaw=tempdata,
                                    signal="input", response="output",
                                    output_path="minimal_exampleProbs/")
```

The above command generates the following graph in the output directory

Diagnostics

The diagnostic test can be performed as follows

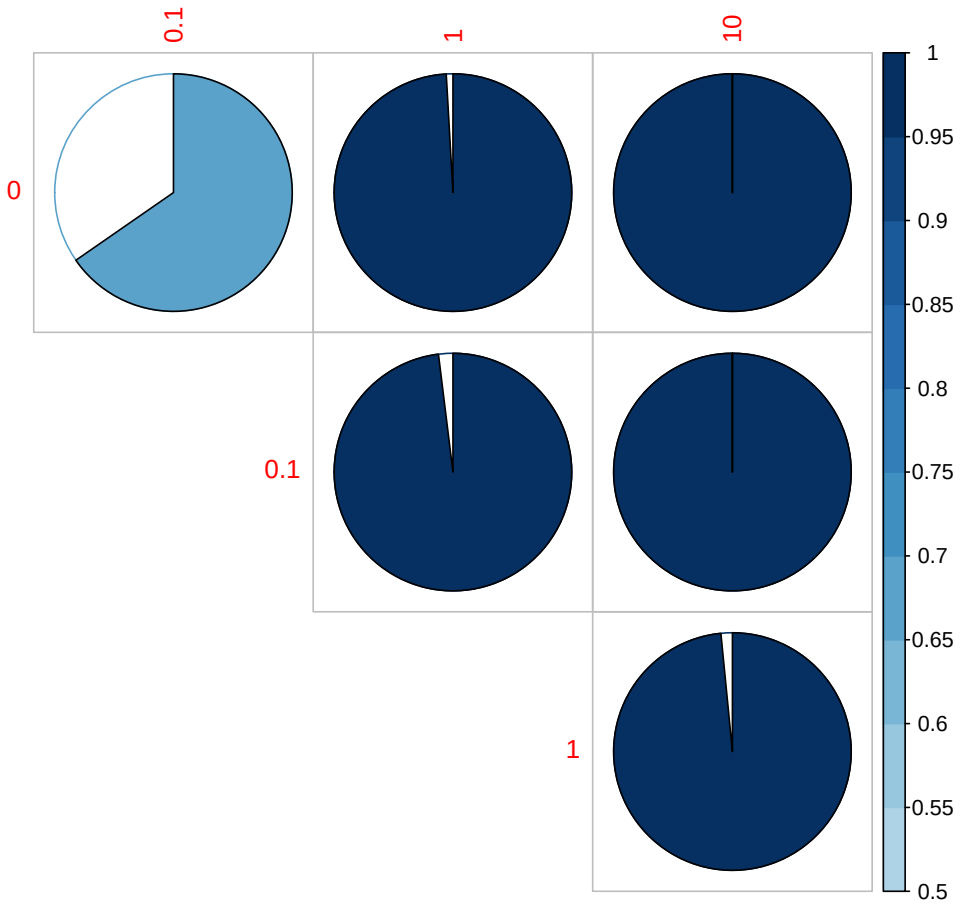


Figure 2: Standard output graph presenting probabilities of correct discrimination between each pair of input values.

```
dir.create("example1_testing/")
outputCLR=capacity_logreg_main(dataRaw=data_example1,
                               signal="signal",response="response",
                               output_path="example1_testing/",
                               testing=TRUE, TestingSeed = 1234, testing_cores = 4,
                               boot_num = 40, boot_prob = 0.8,
                               traintest_num = 40,partition_trainfrac = 0.6)
```

It will run diagnostics with 40 re-sampling of the data, where bootstrap is calculated using 80% of the data, while the over-fitting test uses 60% of the original dataset.

It provides the following result

The top diagram shows the value of the capacity estimate (in black) obtained from the complete dataset and the mean value of bootstrap repetitions with indicated +/- standard deviation (in red). Plots that follow show histograms of calculated capacities for different diagnostic regimes. The black dot represents the estimate of the channel capacity based on the complete dataset. In addition, corresponding empirical p-values of both tests (left- and right-sided) are calculated to assess the randomness of obtained results (PV in the plots).

A reliable estimation of the information capacity should yield the following results of the bootstrap and overfitting tests.

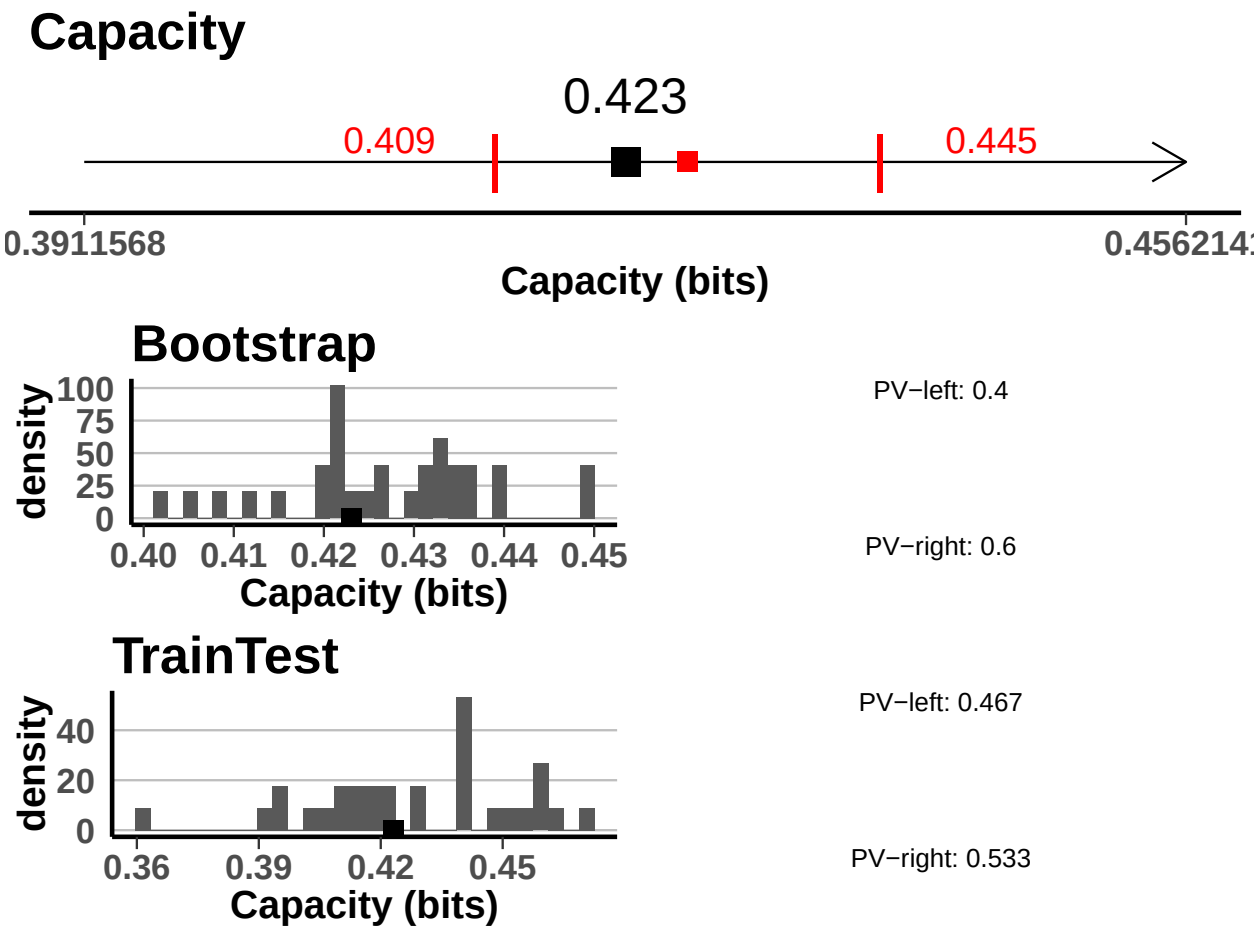


Figure 3: Standard output graph of the diagnostic procedures. P-values (PV) are based on empirical test either left- or right- sided. In the top axis, black dot represents the estimate of the channel capacity that involves the compete dataset, red dot is the mean of bootstrap procedures, while the bars are mean +/- sd. The remaining panels are histograms of all repetitions of a specific diagnostic procedure.

1. The bootstrap test should yield distribution of the capacity estimates with small variance. In addition, the capacity estimated based on the complete dataset should not be an outlier (p-value>0.05). Otherwise, it would indicate that the sample size is too low for an accurate estimation of the channel capacity.
2. The over-fitting test should provide similar results. The capacity estimate obtained based on the complete dataset should lie within the distribution of capacities generated in the test. In the opposite case, it could mean that the logistic regression model does not fully grasp the essential aspects of input-output dependencies in the data.

5.2 Further step-by-step introductory examples

Two step-by-step examples that further illustrate the applicability of the SLEMI package are provided in the Section 6 of the 'testing procedures' pdf file that is part of the package.

5.3 Examples in MP and SI

To reproduce results of the NFkB analysis presented in the MP as well as the results of the comparison with the KNN method presented in the Section 2 of the **SI** see Section 7 of the 'testing procedures' pdf file that is part of the package.

6 List of all package's functions

The list below conatains all functions available to the user:

- `capacity_logreg_main()` - is the main wrapper function that estimates channel capacity based on experimental data
- `capacity_logreg_algorithm()` - implements algorithm to estimate channel capacity using `nnet` package
- `capacity_klogreg_algorithm()` - implements algorithm to estimate channel capacity using `glmnet` package
- `capacity_logreg_testing()` - performs diagnostic procedures
- `capacity_output_graphs()` - generates exploratory graphs
- `mi_logreg_main()` - estimates mutual information
- `prob_discr_pairwise()` - estimates probabilities of discrimination between all pairs of input values
- `formula_generator()` - generates a formula object based on input and output specification
- `sampling_bootstrap()`, `sampling_partition()`, `sampling_shuffle()` - generates subsets of data to use in diagnostic procedures
- `theme_publ()` - changes the visual elements of ggplot object

The tables below contain full specification of the package's functions

Function: `capacity_logreg_main()`
Main wrapper function to perform analysis of channel capacity from experimental data

Arguments

name	description	default
dataRaw	data frame with input (X) and output (Y) values in separate columns	**(required)**
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
output_path	directory in which result and graphs will be saved	**(required)**
scale	logical indicating if preprocessing (centering and scaling) should be carried out before the analysis	`TRUE`
graphs	logical indicating if standard graphs should be created	`TRUE`
model_out	logical indicating if the model object should be returned	`TRUE`
dataout	logical indicating if the dataRaw should be returned with results	`TRUE`
testing	logical indicating if diagnostics should be performed	`FALSE`
TestingSeed	the seed of random number generator to be used in diagnostics	1234
testing_cores	number of cores to use in parallel computing in diagnostics	1
boot_num	the number of bootstrap tests to be performed (used if `testing=TRUE`)	10
boot_prob	the proportion of data to be used in bootstrap (used if `testing=TRUE`)	0.8
traintest_num	the number of over-fitting tests to be performed (used if `testing=TRUE`)	10
partition_trainfrac	the proportion of data to be used as a training dataset (used if `testing=TRUE`)	0.6
side_variables	an optional character vector indicating names of columns in dataRaw with side variables, if `NULL` no side variables are included in estimation	`NULL`
resamp_num	is the number of resmapling tests to be performed (used if `testing=TRUE`)	10
plot_height	the basic dimnesion of plots (height)	4
plot_width	the basic dimnesions of plots (width)	6
cc_maxit	the maximum number of iteration to optimise channel capacity	100
lr_maxit	the maximum number of iteration to estimate logisitic model	1000
maxNWts	the maximum number of parameters in logistic regression algorithm	5000
formula_string	character object that includes a formula syntax to use in logistic model	`NULL`
glmnet_algorithm	logical indicating if the `glmnet` package should be used	`FALSE`
dataMatrix	numeric matrix with columns treated as explanatory variables in logistic model (used if `glmnet_algorithm=TRUE`)	`NULL`
glmnet_cores	the number of cores to use in parallel computing of `glmnet package` (used if `glmnet_algorithm=TRUE`)	1
glmnet_lambdanum	is the lambda parameter as in `glmnet` package (used if `glmnet_algorithm=TRUE`)	10

Values – a list with elements

name	description
cc	a numeric with the estimate of channel capacity (in bits)
p_opt	a numeric vector with estimated optimal input probability
time	processing time of the algorithm
params	a vector of parameters used in the algorithm
data	a data.frame with the raw experimental data (if `dataout=TRUE`)
regression	confusion matrix of logistic regression predictions
model	nnet object describing logistic regression model (if `model_out=TRUE`)
logGraphs	a list of gg or ggtables objects with a standard set of exploratory graphs (if `graphs=TRUE`)
testing	a list of results of diagnostic procedures, e.g. $testing$bootstrap has `boot_num` elements, each with results of the algorithm of each diagnostic run
testing_pv	a list of left- and right-tailed p-values of diagnostic procedures

Function: `mi_logreg_main()`
Main wrapper function to mutual information from experimental data

Arguments

name	description	default
dataRaw	data frame with input (X) and output (Y) values in separate columns	**(required)**
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
output_path	directory in which result and graphs will be saved	**(required)**
scale	logical indicating if preprocessing (centering and scaling) should be carried out before the analysis	`TRUE`
graphs	logical indicating if standard graphs should be created	`TRUE`
model_out	logical indicating if the model object should be returned	`TRUE`
dataout	logical indicating if the dataRaw should be returned with results	`TRUE`
testing	logical indicating if diagnostics should be performed	`FALSE`
TestingSeed	the seed of random number generator to be used in diagnostics	1234
testing_cores	number of cores to use in parallel computing in diagnostics	1
boot_num	the number of bootstrap tests to be performed (used if `testing=TRUE`)	10
boot_prob	the proportion of data to be used in bootstrap (used if `testing=TRUE`)	0.8
traintest_num	the number of over-fitting tests to be performed (used if `testing=TRUE`)	10
partition_trainfrac	the proportion of data to be used as a training dataset (used if `testing=TRUE`)	0.6
side_variables	an optional character vector indicating names of columns in dataRaw with side variables, if `NULL` no side variables are included in estimation	`NULL`
resamp_num	is the number of resmapling tests to be performed (used if `testing=TRUE`)	10
plot_height	the basic dimnesion of plots (height)	4
plot_width	the basic dimnesions of plots (width)	6
pinput	an optional numeric vector with arbitrary probabilities of input. If `NULL`, fractions of observations in full dataset of each class are used.	`NULL`
lr_maxit	the maximum number of iteration to estimate logisitic model	1000
maxNWts	the maximum number of parameters in logistic regression algorithm	5000
formula_string	character object that includes a formula syntax to use in logistic model	`NULL`
glmnet_algorithm	logical indicating if the `glmnet` package should be used	`FALSE`
dataMatrix	numeric matrix with columns treated as explanatory variables in logistic model (used if `glmnet_algorithm=TRUE`)	`NULL`
glmnet_cores	the number of cores to use in parallel computing of `glmnet package` (used if `glmnet_algorithm=TRUE`)	1
glmnet_lambdanum	is the lambda parameter as in `glmnet` package (used if `glmnet_algorithm=TRUE`)	10

Values – a list with elements

name	description
mi	a numeric with the estimate of mutual information (in bits)
p_opt	a numeric vector with estimated optimal input probability
time	processing time of the algorithm
params	a vector of parameters used in the algorithm
data	a data.frame with the raw experimental data (if `dataout=TRUE`)
regression	confusion matrix of logistic regression predictions
model	nnet object describing logistic regression model (if `model_out=TRUE`)
logGraphs	a list of gg or ggtables objects with a standard set of exploratory graphs (if `graphs=TRUE`)
testing	a list of results of diagnostic procedures, e.g. $testing$bootstrap has `boot_num` elements, each with results of the algorithm of each diagnostic run
testing_pv	a list of left- and right-tailed p-values of diagnostic procedures

Function: `prob_discr_pairwise()`
Computation of pairwise probabilities of discrimination

Arguments

name	description	default
dataRaw	data frame with input (X) and output (Y) values in separate columns	**(required)**
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
output_path	directory in which result and graphs will be saved	**(required)**
scale	logical indicating if preprocessing (centering and scaling) should be carried out before the analysis	`TRUE`
model_out	logical indicating if the model object should be returned	`TRUE`
side_variables	an optional character vector indicating names of columns in dataRaw with side variables, if `NULL` no side variables are included in estimation	`NULL`
lr_maxit	the maximum number of iteration to estimate logisitic model	1000
maxNWts	the maximum number of parameters in logistic regression algorithm	5000
formula_string	character object that includes a formula syntax to use in logistic model	`NULL`

Values – a graph of pie charts is created in `output_path` directory.
In addition, function returns a list with elements

name	description
prob_matr	a symmetric numeric matrix of size `length(unique(dataRaw[[signal]]))`×`length(unique(dataRaw[[signal]]))` with probability of discriminating between i-th and j-th input values in [i,j] cell
model	a list of nnet objects describing logistic regression models (if `model_out=TRUE`)

Function: `capacity_logreg_algorithm()`
Implements algorithm to estimate channel capacity using `nnet` package

Arguments

name	description	default
data	data frame with input (X) and output (Y) values in separate columns	**(required)**
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
model_out	logical indicating if the model object should be returned	`TRUE`
side_variables	an optional character vector indicating names of columns in dataRaw with side variables, if `NULL` no side variables are included in estimation	`NULL`
cc_maxit	the maximum number of iteration to optimise channel capacity	100
lr_maxit	the maximum number of iteration to estimate logisitic model	1000
maxNWts	the maximum number of parameters in logistic regression algorithm	5000
formula_string	character object that includes a formula syntax to use in logistic model	`NULL`

Values – a list with elements

name	description
cc	a numeric with the estimate of channel capacity (in bits)
p_opt	a numeric vector with estimated optimal input probability
regression	confusion matrix of logistic regression predictions
model	`nnet` object describing logistic regression model (if `model_out=TRUE`)

Function: `capacity_klogreg_algorithm()`
Implements algorithm to estimate channel capacity using `glmnet` package

Arguments

name	description	default
dataMatrix	numeric matrix with columns treated as explanatory variables (output, Y, of the channel)	**(required)**
dataSignal	factor vector with inputs (X) of the channel length must be equal to the number of rows of dataMatrix	**(required)**
cv_core_num	the number of cores to use in parallel computing of `glmnet package`	1
lambda_num	is the lambda parameter as in `glmnet` package	10
model_out	logical indicating if the model object should be returned	`TRUE`
cc_maxit	the maximum number of iteration to optimise channel capacity	100

Values – a list with elements

name	description
cc	a numeric with the estimate of channel capacity (in bits)
p_opt	a numeric vector with estimated optimal input probability
regression	confusion matrix of logistic regression predictions
model	`glmnet` object describing logistic regression model (if `model_out=TRUE`)

Function: `capacity_logreg_testing()`
Performs diagnostic procedures

Arguments		
name	description	default
data	data frame with input (X) and output (Y) values in separate columns	**(required)**
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
output_path	directory in which result and graphs will be saved	**(required)**
TestingSeed	the seed of random number generator to be used in diagnostics	1234
testing_cores	number of cores to use in parallel computing in diagnostics	1
boot_num	the number of bootstrap tests to be performed (used if `testing=TRUE`)	10
boot_prob	the proportion of data to be used in bootstrap (used if `testing=TRUE`)	0.8
traintest_num	the number of over-fitting tests to be performed (used if `testing=TRUE`)	10
partition_trainfrac	the proportion of data to be used as a training dataset (used if `testing=TRUE`)	0.6
side_variables	an optional character vector indicating names of columns in dataRaw with side variables, if `NULL` no side variables are included in estimation	`NULL`
resamp_num	is the number of resmapling tests to be performed (used if `testing=TRUE`)	10
cc_maxit	the maximum number of iteration to optimise channel capacity	100
lr_maxit	the maximum number of iteration to estimate logisitic model	1000
maxNWts	the maximum number of parameters in logistic regression algorithm	5000
formula_string	character object that includes a formula syntax to use in logistic model	`NULL`
glmnet_algorithm	logical indicating if the `glmnet` package should be used	`FALSE`
dataMatrix	numeric matrix with columns treated as explanatory variables in logistic model (used if `glmnet_algorithm=TRUE`)	`NULL`
glmnet_cores	the number of cores to use in parallel computing of `glmnet package` (used if `glmnet_algorithm=TRUE`)	1
glmnet_lambdanum	is the lambda parameter as in `glmnet` package (used if `glmnet_algorithm=TRUE`)	10
Values – a list with elements		
bootstrap	list of size `boot_num`, where each element is the returned value of `capacity_logreg_algorithm()` from a single run of bootstrap	
traintest	list of size `traintest_num`, where each element is the returned value of `capacity_logreg_algorithm()` from a single run of over-fitting test	
resamplingMorph	list of size `resamp_num`, where each element is the returned value of `capacity_logreg_algorithm()` from a single run of resampling test (used if `side_variables` is not `NULL`)	
bootResampMorph	list of size `resamp_num`, where each element is the returned value of `capacity_logreg_algorithm()` from a single run of resampling test II (used if `side_variables` is not `NULL`)	

Function: `capacity_output_graphs()`
Generates exploratory graphs

Arguments		
name	description	default
data	data frame with input (X) and output (Y) values in separate columns	**(required)**
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
output_path	directory in which result and graphs will be saved	**(required)**
cc_output	logical indicating if preprocessing (centering and scaling)	`TRUE`
height	the basic dimnesion of plots (height)	4
width	the basic dimnesions of plots (width)	6

Values – a list with elements	
name	description
1	A comprehensive summary plot
2	Input-Output relation
3	Boxplots of data
4	Violin plots of data
5	Histograms of data
6	Boxplot of side variables in data
7	Capacity results
8	Density plots
9	A simple summary plot

Function: `formula_generator()`
Generates a formula object based on input and output specification

Arguments		
name	description	default
signal	character indicating a name of column of dataRaw with input (X)	**(required)**
response	character vector indicating names of columns of dataRaw with measurements of outputs (Y)	**(required)**
side_variables	an optional character vector indicating names of columns in dataRaw with side variables, if `NULL` no side variables are included in estimation	`NULL`
Values – a list with elements		
name	description	
formula_string	character object that includes a formula syntax to use in logistic model	`NULL`

Function: `sampling_bootstrap()`, `sampling_partition()`, `sampling_shuffle()`
Used to generate subsets of data to use in diagnostic procedures

Arguments		
name	description	default
data	data.frame to be resampled	**(required)**
dataDiv	character indicating column of data, with respect to which split the data; only in `sampling_bootstrap()` and `sampling_partition()`	**(required)**
prob	the of data that should be sampled from the whole dataset; only in `sampling_bootstrap()`	**(required)**
partition_trainfrac	the proportion of data to be used as a training dataset; only in `sampling_partition()`	**(required)**
side_variables	vector of characters indicating columns of data the will be reshuffled; only in `sampling_shuffle()`	**(required)**
Values – a data.frame with the same structure as initial data object		

Function: `theme_publ()`
Changes the visual elements of ggplot object

Arguments		
name	description	default
version	possible values: 1,2,3. Selects different coloring and presentation options	1
base_size	the size of font to use in graph	12
base_family	the type of font to use in graph	sans
Values – a ggplot theme object		