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

User Manual

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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.

Importantly, 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.

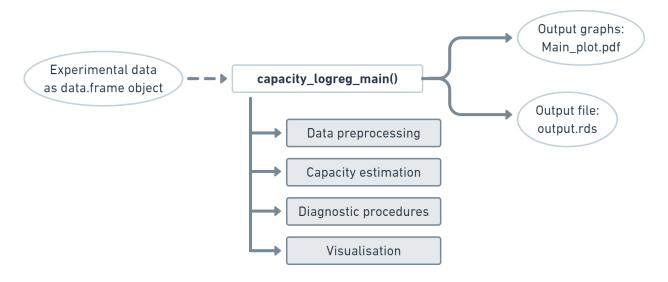


Figure 1: Main function to estimate channel capacity

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 within 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 an internal function capacity_logreg_testing(). These are based on data bootstrapping and overfitting test.

For visualization, a set of graphs is created by an internal function <code>capacity_output_graphs()</code> and saved in a specified directory. In addition, <code>capacity_logreg_main()</code> 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 requires the input distribution to be specified bythe user as a function's argument.

Logistic regression and Monte Carlo methods, following an analogous algorithm as within the capacity_logreg_algorithm() function, 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 (internal functions capacity_output_graphs() and capacity_logreg_testing()).

The prob_discr_pairwise() allows to estimate probabilities of correct 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. The probabilities of correct discrimination are visualized with a graph composed of pie charts.

input	output 1	output 2	output 3	
$n_1 \left\{ \begin{array}{c} x_1 \\ \vdots \\ x_1 \end{array} \right.$	$y_{1,1}^1$ \vdots $y_{n_1,1}^1$	$y_{1,2}^1 \\ \vdots \\ y_{n_1,2}^1$	$\begin{bmatrix} y_{1,m}^1 \\ \vdots \\ y_{n_1,m}^1 \end{bmatrix}$	
$n_2 \left\{ \begin{array}{c} x_2 \\ \vdots \\ x_2 \end{array} \right.$	$y_{1,1}^2$ \vdots $y_{n_2,1}^2$	$y_{n_{1},2}^{1}$ $y_{1,2}^{2}$ \vdots $y_{n_{2},2}^{2}$	$y_{n_1,m}^1$ $y_{1,m}^2$ \vdots $y_{n_2,m}^2$	
:	i :	÷	i :	•••
$n_m \left\{ \begin{array}{c} x_m \\ \vdots \\ x_m \end{array} \right.$	$\begin{array}{c c} y_{1,1}^m \\ \vdots \\ y_{n_m,1}^m \end{array}$	$y_{1,2}^m \\ \vdots \\ y_{n_m,2}^m$	$\begin{bmatrix} y_{1,m}^m \\ \vdots \\ y_{n_m,m}^m \end{bmatrix}$	

Figure 2: Conceptual representation of a generic experimental dataset needed for quantifying information transmission of a channel

2.1 Input data

Functions mi_logreg_main(), capacity_logreg_main(), prob_discr_pairwise() require data in the form of the object data.frame with a specific 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

Therefore, the input data frame is expected to have the form represented 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); these 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	100 ng	1.3534083	3.0158004	5.1592848
11541	100 ng	1.7007936	2.2224497	3.5463418
11542	100 ng	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 6

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

- 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 data_out=TRUE)
- time processing time of the algorithm
- params a vector of parameters used in the algorithm
- regression a confusion matrix of logistic regression predictions

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 for calculation of the mutual information. It is done 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.

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 the 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)
- diagnostics a list of summaries describing fitted logistic regression models of classification between each pair of 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 the sole calculation of the information capacity, the function <code>capacity_logreg_main()</code> can also be used to asses accuracy of the channel capacity estimates resulting from potentially insuffecient sample size and potential over-fitting of the regression model. Two test are implemented. Precisely, the function can perform

- 1. Bootstrap test capacity is re-calculated using $\alpha\%$ of data, sampled from the original dataset without replacement. After repeating the procedure n times, standard deviation of the obtained sample can serve as an error of the 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 by changing 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 <code>capacity_logreg_main()</code> 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
- 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

The generated data frame has the following structure

	input	output
1	0	-0.2447518
2	0	-0.5217063
2001	1	5.3107607
2002	1	5.2957607
3999	10	7.8274830
4000	10	9.5975094

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

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)

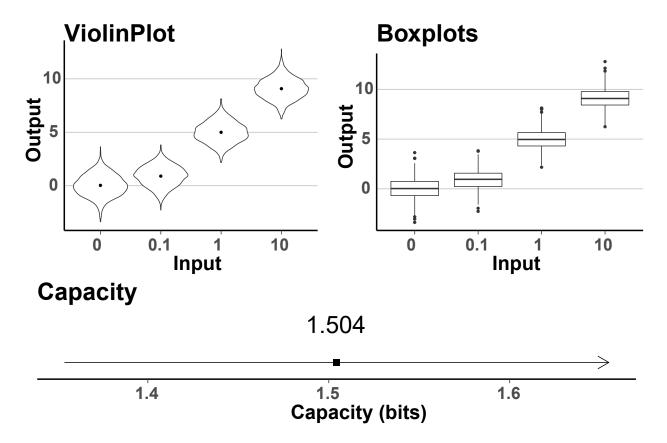


Figure 3: Standard output graph of the minimal working example

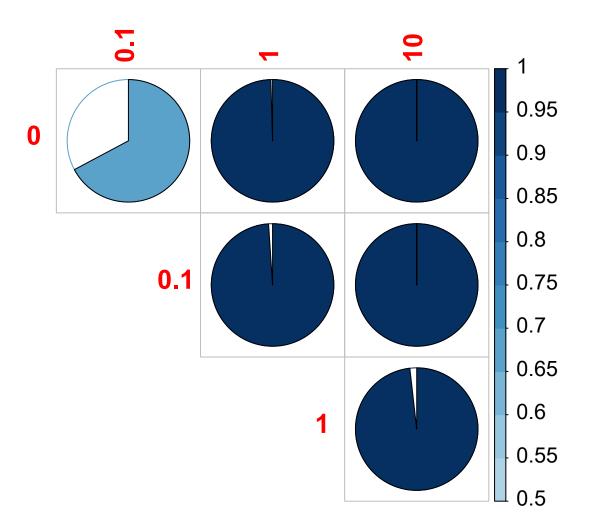


Figure 4: Standard output graph presenting probabilities of correct discrimination between each pair of input values.

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

and display results

[1] "Mutual Information: 1.48915671813912; Channel Capacity: 1.54047606466259"

Calculation of the probabilities of correct discrimination

Probabilities of correct discrimination between input values are calculated as follows

The above command generates graph shown in Figure 4 in the output directory

Diagnostics

The diagnostic test can be performed as follows

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.

Its results are provided in graph presented in Figure 5.

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.

- 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.

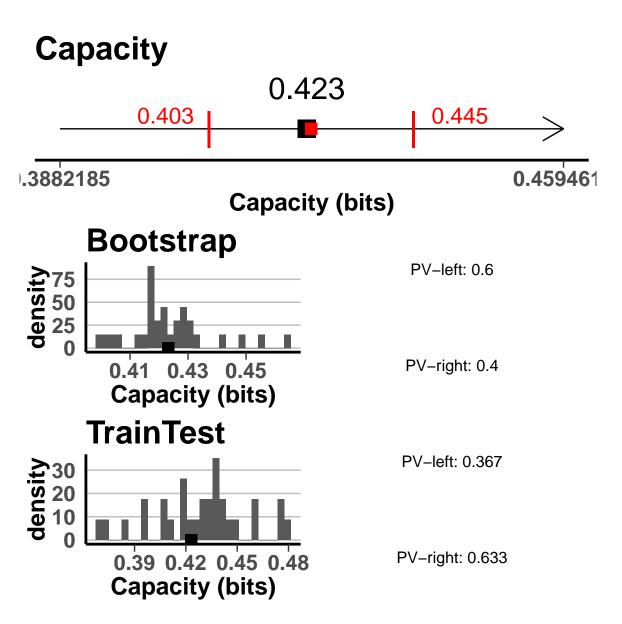


Figure 5: Standard output graph of the diagnostic procedures. P-values (PV) are based on empirical test either left- or right- sided. In the top axis, black dot represents the estimate of the channel capacity that involves the compete dataset, red dot is the mean of bootstrap procedures, while the bars are mean +/- sd. The remaining panels are histograms of all repetitions of a specific diagnostic procedure.

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 contains 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
- mi_logreg_main() estimates mutual information
- mi_logreg_algorithm() implements algorithm to estimate mutual information using nnet package
- prob_discr_pairwise() estimates probabilities of discrimination between all pairs of input values

All other functionalities (graphs, testing procedures) are managed by internal functions. 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	(required)
	with measurements of outputs (Y)	
$output_path$	directory in which result and graphs will be saved	(required)
scale	logical indicating if preprocessing (centering and scaling)	TRUE
	should be carried out before the analysis	
${ m model_out}$	logical indicating if the model object should be returned	TRUE
$data_out$	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	10
	(used if testing=TRUE)	
$boot_prob$	the proportion of data to be used in bootstrap	0.8
	(used if testing=TRUE)	
$traintest_num$	the number of over-fitting tests to be performed	10
	(used if testing=TRUE)	
partition_trainfrac	the proportion of data to be used as a training dataset	0.6
	(used if testing=TRUE)	
$side_variables$	an optional character vector indicating names of columns in dataRaw	NULL
	with side variables, if NULL no side variables are included in estimation	
$sidevar_num$	is the number of resmapling tests to be performed	10
	(used if testing=TRUE)	
$plot_height$	the basic dimnesion of plots (height)	4
$\operatorname{plot}_{\operatorname{\!-}\!\operatorname{\!-}}$	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
$\max NWts$	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	
= -		

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 numeric vector with estimated optimal input probability time processing time of the algorithm a vector of parameters used in the algorithm data (if dataout=TRUE) regression predictions model (if model_out=TRUE) 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

Train wrapper rain	Arguments	
namo	description	default
name 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	(required)
output noth	with measurements of outputs (Y)	(maguinad)
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
${ m model_out}$	logical indicating if the model object should be returned	TRUE
${ m data_out}$	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	10
	(used if testing=TRUE)	
boot_prob	the proportion of data to be used in bootstrap	0.8
1	(used if testing=TRUE)	
$traintest_num$	the number of over-fitting tests to be performed	10
	(used if testing=TRUE)	
partition_trainfrac	the proportion of data to be used as a training dataset	0.6
	(used if testing=TRUE)	
side_variables	an optional character vector indicating names of columns in dataRaw	NULL
	with side variables, if NULL no side variables are included in estimation	
sidevar_num	is the number of resmapling tests to be performed	10
	(used if testing=TRUE)	
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.	NULL
1 1	If NULL, fractions of observations in full dataset of each class are used.	
lr_maxit	the maximum number of iteration to estimate logisitic model	1000
$\max NWts$	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
0	Values – a list with elements	
name	description	
mi	a numeric with the estimate of mutual information (in bits)	
pinput	a numeric vector with prior probabilities of input	
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)	
testing	a list of results of diagnostic procedures, e.g. \$testing\$bootstrap	
J	has boot_num elements, each with results of the algorithm of each diagno	stic run
	,	

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	(required)	
	with measurements of outputs (Y)		
$\operatorname{output_path}$	directory in which result and graphs will be saved	(required)	
scale	logical indicating if preprocessing (centering and scaling)	TRUE	
	should be carried out before the analysis		
diagnostics	is a logical indicating if details of logistic regression fitting should	TRUE	
	be included in output list		
$side_variables$	an optional character vector indicating names of columns in dataRaw	NULL	
	with side variables, if NULL no side variables are included in estimation		
lr_maxit	the maximum number of iteration to estimate logisitic model	1000	
$\max NWts$	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[[sig	nal]]))	
with probability of discriminating between i-th and j-th input values in [i,			
diagnostics	diagnostics a list of diagnostics summaries that correspond to logistic regression models		
	fitted for each pair of input values (if diagnostics=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	(required)	
	with measurements of outputs (Y)		
$model_out$	logical indicating if the model object should be returned	TRUE	
$side_variables$	an optional character vector indicating names of columns in dataRaw	NULL	
	with side variables, if NULL no side variables are included in estimation		
cc_maxit	the maximum number of iteration to optimise channel capacity	100	
lr_maxit	the maximum number of iteration to estimate logisitic model	1000	
$\max NWts$	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)		
$\mathrm{p_opt}$	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: mi_logreg_algorithm()
Implements algorithm to estimate mutual information using nnet package

	0 1 0		
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	(required)	
	with measurements of outputs (Y)		
$model_out$	logical indicating if the model object should be returned	TRUE	
$side_variables$	an optional character vector indicating names of columns in dataRaw	NULL	
	with side variables, if NULL no side variables are included in estimation		
lr_maxit	the maximum number of iteration to estimate logisitic model	1000	
$\max NWts$	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		
mi	a numeric with the estimate of mutual information (in bits)		
pinput	a numeric vector with prior probabilities of input		
regression	confusion matrix of logistic regression predictions		
model	model nnet object describing logistic regression model (if model_out=TRUE)		