Package 'MaxWiK'

July 7, 2025

Title Machine Learning Method Based on Isolation Kernel Mean Embedding

Version 1.0.6

Description Incorporates Approximate Bayesian Computation to get a posterior distribution and to select a model optimal parameter for an observation point. Additionally, the meta-sampling heuristic algorithm is realized for parameter estimation, which requires no model runs and is dimension-independent. A sampling scheme is also presented that allows model runs and uses the meta-sampling for point generation. A predictor is realized as the meta-sampling for the model output. All the algorithms leverage a machine learning method utilizing the maxima weighted Isolation Kernel approach, or 'MaxWiK'. The method involves transforming raw data to a Hilbert space (mapping) and measuring the similarity between simulated points and the maxima weighted Isolation Kernel mapping corresponding to the observation point. Comprehensive details of the methodology can be found in the papers Iurii Nagornov (2024) <doi:10.1007/978-3-031-66431-1_16> and Iurii Nagornov (2023) <doi:10.1007/978-3-031-29168-5_18>.

License GPL (>= 3)

Depends R (>= 3.3.0)

Imports methods, stats, utils, scales, parallel, abc, ggplot2

Suggests rmarkdown, knitr

Encoding UTF-8

RoxygenNote 7.3.2

VignetteBuilder knitr

LazyData true

NeedsCompilation no

Author Yuri Nagornov [aut, cre, cph] (ORCID: <https://orcid.org/0000-0002-7935-6776>)

Maintainer Yuri Nagornov <nagornov.yuri@gmail.com>

Repository CRAN

Date/Publication 2025-07-07 05:30:02 UTC

Contents

`apply_range` *Function to restrict values of the data according with the range for each dimension*

Description

Function to restrict values of the data according with the range for each dimension

Usage

```
apply_range(diapason, input.data)
```

Arguments

`diapason`	Vector of min and max values or data frame with two rows (min and max) for each dimension of input data
`input.data`	Data frame of input where values will be corrected

Value

The same data frame with corrected values according to the diapason

Examples

```
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the templates and vignettes for usage.
```

Data.2D *List of the objects for the 2D example of the MaxWiK methods usage*

Description

A list containing input and output data for 2D example for Approximate Bayesian Computation, including sampling scheme, meta-sampling, and prediction. To understand all details of the dataset, please, be kind to see vignette of the package.

Usage

```
Data.2D
```

Format

A list of:

X Input data frame of the model

Y Output data frame of the model

observation Data frame with observation info

ABC List of hyperparameters, the matrix of Voronoi sites, posteriori distribution, and results of MaxWiK algorithm

metasampling List of results of meta-sampling algorithm, and the network of points during meta-sampling

sampling List of object which are necessary for sampling algorithm like function for simulation, parameters of the model, MSE (mean squared error), and X12 - generated points

predictor List of object which are necessary for predictor algorithm like posteriori.MaxWiK, result of the algorithm, and network of points during meta-sampling

MaxWiK.ggplot.density *Density plot*

Description

Density plot

Usage

```
MaxWiK.ggplot.density(
  title = "",
  datafr1,
  datafr2,
  var.df,
  obs.true = NULL,
  best.sim = NULL,
  clrs = c("#a9b322", "#f9b3a2", "red", "blue"),
  alpha = c(0.1, 0.4),
  lw = c(0.7, 0.7),
  lt = c("dashed", "dotted")
)
```

Arguments

title	Title of the plot
datafr1	data frame 1
datafr2	data frame 2
var.df	Variables to show
obs.true	True observation if so, NULL by default
best.sim	The best point from a simulation if so, NULL by default
clrs	Colors to plot, by default it is c("#a9b322", "#f9b3a2", 'red', 'blue')
alpha	Transparency values for density plots
lw	Line widths
lt	Line types

Value

Make and return the ggplot object of the densities of the data frames

Examples

```
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the templates and vignettes for usage.
# Function 'MaxWiK.ggplot.density()' is used in the MaxWiK.ABC.R and
# MaxWiK.Predictor.R templates.
```

MaxWiK_templates *Function to copy the templates from extdata folder in the library to /Templates/ folder in the working directory*

Description

Function to copy the templates from extdata folder in the library to /Templates/ folder in the working directory

Usage

```
MaxWiK_templates(dir)
```

Arguments

dir	Folder to where files should be save, by default dir = './'

Value

List of logic numbers for each copied file, TRUE - success, FALSE - not success

Examples

```
MaxWiK_templates( dir = tempdir() )
```

---

meta_sampling *Function to get Approximate Bayesian Computation based on Maxima Weighted Isolation Kernel mapping*

Description

The function `meta_sampling()` iteratively generates tracer based on the simple procedure:

- making a reflection of the top points from the best point,
- and then generating the point tracers between them,
- finally, the algorithm chooses again the top points and the best point (`sudoku()` function is used),
- repeat all the steps until condition to be `TRUE`:
  `abs( min( sim_tracers ) - sim_previous ) < epsilon`

The function `MaxWiK.predictor()` uses the meta-sampling for a prediction

The function `get.MaxWiK()` is used to get Approximate Bayesian Computation based on Maxima Weighted Isolation Kernel mapping. On given data frame of parameters, statistics of the simulations and an observation, using the internal parameters psi and t, the function `get.MaxWiK()` returns the estimation of a parameter corresponding to Maxima weighted Isolation Kernel ABC method.

Usage

```
meta_sampling(
  psi = 4,
  t = 35,
  param,
  stat.sim,
  stat.obs,
```

```
  talkative = FALSE,
  check_pos_def = FALSE,
  n_bullets = 16,
  n_best = 10,
  halfwidth = 0.5,
  epsilon = 0.001,
  rate = 0.1,
  max_iteration = 15,
  save_web = TRUE,
  use.iKernelABC = NULL
)

MaxWiK.predictor(
  psi = 4,
  t = 35,
  param,
  stat.sim,
  new.param,
  talkative = FALSE,
  check_pos_def = FALSE,
  n_bullets = 16,
  n_best = 10,
  halfwidth = 0.5,
  epsilon = 0.001,
  rate = 0.1,
  max_iteration = 15,
  save_web = TRUE,
  use.iKernelABC = NULL
)

get.MaxWiK(
  psi = 40,
  t = 350,
  param,
  stat.sim,
  stat.obs,
  talkative = FALSE,
  check_pos_def = TRUE,
  Matrix_Voronoi = NULL
)
```

Arguments

psi	Integer number. Size of each Voronoi diagram or number of areas/points in the Voronoi diagrams
t	Integer number of trees in the Isolation Forest
param	or par.sim - data frame of parameters of the model
stat.sim	Summary statistics of the simulations (model output)

stat.obs	Summary statistics of the observation point
talkative	Logical parameter to print or do not print messages
check_pos_def	Logical parameter to check the Gram matrix is positive definite or do not check
n_bullets	Number of generating points between two
n_best	Number of the best points to construct the next web net
halfwidth	Parameter for the algorithm of deleting of generated points
epsilon	Criterion to stop meta-sampling
rate	Rate to renew points in the web net of generated points
max_iteration	Maximum of iterations during meta-sampling
save_web	Logical to save all the generated points (web net)
use.iKernelABC	The iKernelABC object to use for meta-sampling. By default it is NULL and is generated.
new.param	New parameter for the predictor input
Matrix_Voronoi	is a predefined matrix of information about Voronoi trees (rows - trees, columns - Voronoi points/areas IDs). By default it is NULL and is generated randomly.

Value

The function meta_sampling() returns the list of the next objects:

- input.parameters that is the list of all the input parameters for Isolation Kernel ABC method;
- iteration that is iteration value when algorithm stopped;
- network that is network points when algorithm stopped;
- par.best that is data frame of one point that is the best from all the generated tracer points;
- sim.best that is numeric value of the similarity of the best tracer point;
- iKernelABC that is result of the function get.MaxWiK() given on input parameters;
- spiderweb that is the list of all the networks during the meta-sampling.

The function MaxWiK.predictor() returns the list of the next objects:

- input.parameters that is the list of all the input parameters for Isolation Kernel ABC method;
- iteration that is iteration value when algorithm stopped;
- network that is network points when algorithm stopped;
- prediction.best that is data frame of one point that is the best from all the generated tracer points;
- sim.best that is numeric value of the similarity of the best tracer point;
- iKernelABC that is result of the function get.MaxWiK() given on input parameters;
- spiderweb that is the list of all the networks during the meta-sampling.

The function get.MaxWiK() returns the list of :

- kernel_mean_embedding is a maxima weighted kernel mean embedding (mapping) related to the observation point;

- parameters_Matrix_Voronoi is a matrix of information about Voronoi trees (rows - trees, columns - Voronoi points/areas IDs) for parameters data set;
- parameters_Matrix_iKernel is a matrix of of all points of PARAMETERS in a Hilbert space (rows - points, columns - isolation trees);
- Hilbert_weights is a weights in Hilbert space to get maxima weighted kernel mean embedding for parameters_Matrix_iKernel;
- Matrix_iKernel is a matrix of all points of simulations in a Hilbert space (rows - points, columns - isolation trees);
- iFeature_point is a feature embedding mapping for the OBSERVATION point;
- similarity is a vector of similarities between the simulation points and observation point;
- Matrix_Voronoi is a matrix of information about Voronoi trees (rows - trees, columns - Voronoi points/areas IDs);
- t is a number of trees in the Isolation Forest;
- psi is a number of areas/points in the Voronoi diagrams

Functions

- `meta_sampling()`: The function to get the best value of parameter corresponding to Maxima Weighted Isolation Kernel mapping which is related to an observation point
- `MaxWiK.predictor()`: The function to get the prediction of output based on a new parameter and MaxWiK

Examples

```
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the template 'MaxWiK.ABC.R' and
# vignettes for usage.
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the template 'MaxWiK.Predictor.R'
# and vignettes for usage.
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the template 'MaxWiK.ABC.R' and
# vignettes for usage.
```

---

read_file *Function to read file*

Description

Function to read file

Usage

```
read_file(file_name = "", stringsAsFactors = FALSE, header = TRUE)
```

Arguments

file_name	Name of file to read
stringsAsFactors	Parameter for read.table function, by default stringsAsFactors = FALSE
header	Logical type to read or do not read head of a file

Value

data.frame of data from a file

Examples

```
NULL
```

---

read_hyperparameters *Function to read hyperparameters and their values from the file*

Description

Function to read hyperparameters and their values from the file

Usage

```
read_hyperparameters(input)
```

Arguments

input	File name to input

Value

Parameters and their values

Examples

```
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the templates and vignettes for usage.
```

restrict_data *Function to restrict data in the size to accelerate the calculations*

Description

`restrict_data()` is based on rejection ABC method to restrict original dataset

Usage

```
restrict_data(par.sim, stat.sim, stat.obs, size = 300)
```

Arguments

`par.sim`	Data frame of parameters
`stat.sim`	Data frame of outputs of simulations
`stat.obs`	Data frame of observation point
`size`	Integer number of points to leave from original dataset

Value

`restrict_data()` returns the list of:
par.sim - restricted parameters which are close to observation point
stat.sim - restricted stat.sim which are close to observation point

Examples

```
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the templates and vignettes for usage.
```

sampler_MaxWiK *Function to generate parameters and simulate a model based on MaxWiK algorithm*

Description

Function to generate parameters and simulate a model based on MaxWiK algorithm

Usage

```
sampler_MaxWiK(
  stat.obs,
  stat.sim,
  par.sim,
  model,
  arg0 = list(),
  size = 500,
```

```
  psi_t,
  epsilon,
  nmax = 100,
  include_top = FALSE,
  slowly = FALSE,
  rate = 0.2,
  n_simulation_stop = NA,
  check_err = TRUE,
  include_web_rings = TRUE,
  number_of_nodes_in_ring = 2
)

sampler_MaxWiK_parallel(
  stat.obs,
  stat.sim,
  par.sim,
  model,
  arg0 = list(),
  size = 500,
  psi_t,
  epsilon,
  nmax = 100,
  include_top = FALSE,
  slowly = FALSE,
  rate = 0.2,
  n_simulation_stop = NA,
  check_err = TRUE,
  include_web_rings = TRUE,
  number_of_nodes_in_ring = 2,
  cores = 4
)
```

Arguments

`stat.obs`	Summary statistics of the observation point
`stat.sim`	Summary statistics of the simulations (model output)
`par.sim`	Data frame of parameters of the model
`model`	Function to get output of simulation during sampling
`arg0`	List with arguments for a model function, so that arg0 is NOT changed during sampling
`size`	Number of points in the simulation based on MaxWiK algorithm
`psi_t`	Vector of psi and t hyperparameters.
`epsilon`	Criterion to stop simulation when `MSE_current - MSE_previous < epsilon`
`nmax`	Maximal number of iterations
`include_top`	Logical to include top points (network) from `spider_web()` function to simulate or do not

slowly	Logical for two algorithms: slow and fast seekers in sampling
rate	Rate value in the range [0,1] to define the rate of changing in the original top of sampled points for slow scheme (if slowly = TRUE)
n_simulation_stop	Maximal number of simulations to stop sampling. If n_simulation_stop = NA then there is no restriction (by default)
check_err	Logical parameter to check epsilon or do not
include_web_rings	Logical to include or do not include the cobweb rings to the simulations
number_of_nodes_in_ring	Number of points/nodes between two points in the web ring. By default number_of_nodes_in_ring = 2
cores	Number of cores for parallel calculations of a model (4 by default)

Value

sampler_MaxWiK() returns the list:

- results: results of all the simulations;
- best: the best value of parameter;
- MSE_min: minimum of MSE;
- number_of_iterations: number of iterations;
- time: time of sampling in seconds,
- n_simulations: the total number of simulations.

sampler_MaxWiK_parallel() returns the same output as in sampler_MaxWiK().

Functions

- sampler_MaxWiK_parallel(): Function to generate parameters and simulate a model based on MaxWiK algorithm

Examples

```
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the template 'MaxWiK.Sampling.R'
# and vignettes for usage.
MaxWiK::MaxWiK_templates(dir = tempdir()) # See the template 'MaxWiK.Sampling.R'
# and vignettes for usage. For parallel implementation
# change the function 'sampler_MaxWiK()' to 'sampler_MaxWiK_parallel()'.
```

Index