

Package ‘flimo’

April 2, 2022

Type Package

Title Fixed Landscape Inference MethOd

Version 0.1.1

Author Sylvain Moinard

Maintainer Sylvain Moinard <sylvain.moinard@univ-grenoble-alpes.fr>

Description Likelihood-free inference method for stochastic models.

Uses a deterministic optimizer on simple simulations of the model that are performed with a prior drawn randomness by applying the inverse transform method. Is designed to work on its own and also by using the Julia package Jflimo. See the git page of the project : <<https://metabarcoding.org/flimo>>.

Imports ggplot2, gridExtra, JuliaConnector

License CeCILL

Encoding UTF-8

RoxygenNote 7.1.2

SystemRequirements Julia >= 1.0

VignetteBuilder knitr

Suggests knitr, rmarkdown

NeedsCompilation no

Repository CRAN

Date/Publication 2022-04-01 23:40:06 UTC

R topics documented:

| | |
|-----------------------------|----|
| check_simulator | 2 |
| flimobjective | 3 |
| flimoptim | 4 |
| flimoptim_Julia | 6 |
| flimoptim_R | 8 |
| julia_load | 10 |
| julia_setup | 10 |
| plot.flimo_result | 11 |

| | |
|--------------------------------|----|
| plot_objective | 12 |
| print.flimo_result | 13 |
| summary.flimo_result | 14 |

| | |
|--------------|-----------|
| Index | 15 |
|--------------|-----------|

| | |
|-----------------|------------------------|
| check_simulator | <i>check_simulator</i> |
|-----------------|------------------------|

Description

Run simulations to catch random variations. Warning : does not check it formally. Warning : does not check if quantiles are used several times.

Usage

```
check_simulator(
  simulatorQ,
  ndraw,
  Theta_lower = 0,
  Theta_upper = 1,
  ntheta = 5,
  nruns = 3
)
```

Arguments

| | |
|-------------|---|
| simulatorQ | Function of type simulatorQ(Theta, quantiles) where Theta is the parameter set for the simulations and quantiles are drawn in U(0,1). |
| ndraw | Integer. Number of random variables to draw for one simulation of the model. |
| Theta_lower | 1D numeric array. Lower bounds of Theta parameters. |
| Theta_upper | 1D numeric array. Upper bounds of Theta parameters. |
| ntheta | Integer. Number of Theta parameters to test. |
| nruns | Integer. For each Theta, number of simulations to run. |

Value

Boolean. True if no random effect was detected, False else.

Examples

```
simulatorQ <- function(Theta, quantiles){
  qpois(quantiles, lambda = Theta)
}
check_simulator(simulatorQ, 5, Theta_lower = 50, Theta_upper = 150)
```

| | |
|---------------|----------------------|
| flimobjective | <i>flimobjective</i> |
|---------------|----------------------|

Description

Computes the summary statistics between simulations w.r.t. Theta and data. This function is to be minimized by flimoptim.

Usage

```
flimobjective(Theta, quantiles, data, sumstats, simulatorQ)
```

Arguments

| | |
|------------|--|
| Theta | 1D array. parameters for the simulations. |
| quantiles | 2D array containing values following $U(0,1)$. Row number = number of simulations. Column number = number of random variables to draw in one simulation. |
| data | 1D array containing the observations. |
| sumstats | Function computing the distance between simulations and data of form <code>sumstats(simulations, data)</code> where <code>simulations</code> : 2D array and <code>data</code> : 1D array. <code>ncol(simulations) = length(data)</code> mandatory. |
| simulatorQ | Function of type <code>simulatorQ(Theta, quantiles)</code> where <code>Theta</code> is the parameter set for the simulations and <code>quantiles</code> are drawn in $U(0,1)$. See README for details. |

Value

Numeric value. Distance between summary statistics of data and simulations w.r.t. Theta.

Examples

```
quantiles <- matrix(runif(50), nrow = 10)

data <- rep(100, 5)

sumstats <- function(simulations, data){
  mean_simu <- mean(rowMeans(simulations))
  mean_data <- mean(data)
  (mean_simu-mean_data)^2
}

simulatorQ <- function(Theta, quantiles){
  qpois(quantiles, lambda = Theta)
}

flimobjective(100, quantiles, data, sumstats, simulatorQ)
```

 flimoptim

flimoptim

Description

Computes several parameter inferences with R optimizer or Julia optimizer in a full Julia mode. In R mode (default) : L-BFGS-B optimization. In Julia mode : either IPNewton with or without Automatic Differentiation or Brent optimization.

Usage

```
flimoptim(
  data,
  ndraw,
  sumstats,
  simulatorQ,
  obj = NULL,
  nsim = 10,
  ninfer = 1,
  lower = 0,
  upper = 1,
  Theta0 = (lower + upper)/2,
  randomTheta0 = FALSE,
  mode = c("R", "Julia"),
  AD = TRUE,
  method = "",
  maxit = 1000,
  time_lim = NaN,
  factr = 1e+07,
  pgtol = 0,
  xtol = 0,
  ftol = 0,
  gtol = 1e-08,
  reltol = sqrt(.Machine$double.eps),
  abstol = .Machine$double.eps,
  show_trace = FALSE,
  store_trace = FALSE,
  store_quantiles = FALSE,
  par_names = NULL,
  load_julia = FALSE
)
```

Arguments

| | |
|-------|--|
| data | 1D array containing the observations. |
| ndraw | Integer. Number of random variables to draw for one simulation of the model. |

| | |
|--------------|--|
| sumstats | Summary statistics to measure distance between simulations and data. In R mode : R function of type <code>sumstats(simulations, data)</code> where <code>simulations</code> : 2D array and <code>data</code> : 1D array. <code>ncol(simulations) = length(data)</code> mandatory. In Julia mode : a string containing the script of the Julia function <code>sumstats(simulations, data)</code> . The name "sumstats" is mandatory. |
| simulatorQ | Simulator of the stochastic process with fixed quantiles (see README). or a string (in mode "Julia") containing the script of the Julia function <code>simulatorQ(Theta, quantiles)</code> . In Julia mode, the name "simulatorQ" is mandatory. Theta is the parameter set for the simulations and quantiles are drawn in $U(0,1)$. |
| obj | Objective function to minimize. Default : is directly computed from <code>sumstats</code> and <code>simulatorQ</code> . Either an R function of type <code>objective(Theta, quantiles)</code> (in mode "R") or a string (in mode "Julia") containing the script of the Julia function <code>julia_obj(Theta, quantiles)</code> . Warning : could be tricky if mode = "Julia" to call data. In Julia mode, the name "julia_obj" is mandatory. |
| nsim | Integer. Number of simulations to run for each step of the optimization algorithm. Computation time grows linearly with this number. Default to 10. |
| ninfer | Integer. Number of independent inferences to run. Default to 1. |
| lower | 1D array. Lower bounds for parameters. Same length as upper. |
| upper | 1D array. Upper bounds for parameters. Same length as lower. |
| Theta0 | 1D array. Initial values of the parameters. Default : <code>mean(lower, upper)</code> . |
| randomTheta0 | Boolean. If True, Theta0 is randomly drawn between lower and upper bounds. |
| mode | String. "R" (default) or "Julia". See README. |
| AD | Boolean. Only in Julia mode, uses Automatic Differentiation with IPNewton method. Default to true. |
| method | String. In Julia mode, allows to choose the optimization method : "Brent", "IPNewton". Default : IPNewton. |
| maxit | Integer. Max number of iterations during optimization. Default to 1000. |
| time_lim | Float. Time limit in second for each inference. Default to no limit. Not available for R mode and Brent method in Julia mode. |
| fctr | Float. In R-mode : control parameter for L-BFGS-B method in <code>stats::optim</code> . Default to $1e7$. |
| pgtol | Float. In R-mode : control parameter for L-BFGS-B method in <code>stats::optim</code> . Default to 0. |
| xtol | Float. In Julia mode with IPNewton method : <code>xtol</code> option in <code>Optim.Options</code> . Default to 0. |
| ftol | Float. In Julia mode with IPNewton method : <code>ftol</code> option in <code>Optim.Options</code> . |
| gtol | Float. In Julia mode with IPNewton method : <code>gtol</code> option in <code>Optim.Options</code> . Default to $1e-8$. |
| reltol | Float. In Julia mode with Brent method : <code>reltol</code> of <code>Optim.optimize</code> . Default is <code>sqrt(.Machine\$double.eps)</code> , about $1e-8$. |
| abstol | Float. In Julia mode with Brent method : <code>abstol</code> of <code>Optim.optimize</code> . Default is <code>.Machine\$double.eps</code> , about $1e-16$. |

| | |
|-----------------|---|
| show_trace | Boolean. If true, shows standard trace. Default to false. |
| store_trace | Boolean. If true, stores standard trace as an array of strings. Default to false. Not available for R mode. |
| store_quantiles | Boolean. If true, stores every quantiles used for inference, to reproduce the results. Default to false. |
| par_names | vector of names for parameters. Default is "par1", ..., "parn". |
| load_julia | Boolean. If true, run julia_load. It can take few seconds. Default to False. |

Value

Object of class flimo_result (list) (converted from Julia object in Julia mode) containing every information about convergence results.

Examples

```
data <- rep(100, 5)

sumstats <- function(simulations, data){
  mean_simu <- mean(rowMeans(simulations))
  mean_data <- mean(data)
  (mean_simu-mean_data)^2
}

simulatorQ <- function(Theta, quantiles){
  qpois(quantiles, lambda = Theta)
}

flimoptim(data, 5, sumstats, simulatorQ,
  nsim = 10,
  lower = 50,
  upper = 150,
  method = "Brent")
```

flimoptim_Julia

flimoptim_Julia

Description

Computes several parameter inferences with Julia optimizer and either IPNewton with or without Automatic Differentiation or Brent method.

Usage

```

flimoptim_Julia(
    data,
    ndraw,
    sumstats,
    simulatorQ,
    julia_obj = NULL,
    nsim = 10,
    ninfer = 1,
    lower = 0,
    upper = 1,
    Theta0 = (lower + upper)/2,
    randomTheta0 = FALSE,
    AD = TRUE,
    method = "",
    maxit = 1000,
    time_lim = NULL,
    xtol = 0,
    ftol = 0,
    gtol = 1e-08,
    reltol = sqrt(.Machine$double.eps),
    abstol = .Machine$double.eps,
    show_trace = FALSE,
    store_trace = FALSE,
    store_quantiles = FALSE,
    par_names = NULL,
    load_julia = FALSE
)

```

Arguments

| | |
|------------|--|
| data | ID array containing the observations. |
| ndraw | Integer. Number of random variables to draw for one simulation of the model. |
| sumstats | Summary statistics to measure distance between simulations and data. String containing the script of the Julia function <code>sumstats(simulations, data)</code> . The name "sumstats" is mandatory. |
| simulatorQ | Simulator of the stochastic process with fixed quantiles (see README). <code>simulatorQ(Theta, quantiles)</code> . The name "simulatorQ" is mandatory. Theta is the parameter set for the simulations and quantiles are drawn in $U(0,1)$. |
| julia_obj | Objective function to minimize. Default : is directly computed from <code>sumstats</code> and <code>simulatorQ</code> . String containing the script of the Julia function <code>julia_obj(Theta, quantiles)</code> . Warning : can be tricky to call data. The name "julia_obj" is mandatory. |
| nsim | Integer. Number of simulations to run for each step of the optimization algorithm. Computation time grows linearly with this number. Default to 10. |
| ninfer | Integer. Number of independent inferences to run. Default to 1. |

| | |
|-----------------|--|
| lower | 1D array. Lower bounds for parameters. Same length as upper. |
| upper | 1D array. Upper bounds for parameters. Same length as lower. |
| Theta0 | 1D array. Initial values of the parameters. Default : mean(lower, upper). |
| randomTheta0 | Boolean. If True, Theta0 is randomly drawn between lower and upper bounds. |
| AD | Boolean. Only in Julia mod, uses Automatic Differentiation with IPNewton method. Default to true. |
| method | String. Allows to choose the optimization method : "Brent", "IPNewton". Default : IPNewton. |
| maxit | Integer. Max number of iterations during optimization. Default to 1000. |
| time_lim | Float. Time limit in second for each inference. Default to no limit. Not available for Brent method. |
| xtol | Float. With IPNewton method : xtol option in Optim.Options. Default to 0. |
| ftol | Float. With IPNewton method : ftol option in Optim.Options. Default to 0. |
| gtol | Float. With IPNewton method : gtol option in Optim.Options. Default to 1e-8. |
| reltol | Float. With Brent method : reltol of Optim.optimize. Default is sqrt(.Machine\$double.eps), about 1e-8. |
| abstol | Float. With Brent method : abstol of Optim.optimize. Default is .Machine\$double.eps, about 1e-16. |
| show_trace | Boolean. If true, shows standard trace. Default to false. |
| store_trace | Boolean. If true, stores standard trace as an array of strings. Default to false. Not available for R mod. |
| store_quantiles | Boolean. If true, stores every quantiles used for inference, to reproduce the results. Default to false. |
| par_names | vector of names for parameters. Default is "par1", ..., "parn". |
| load_julia | Boolean. If true, run julia_load. It can take few seconds. Default to False. |

Value

Object of class flimo_result (list) converted from Julia object containing every information about convergence results.

flimoptim_R

flimoptim_R

Description

Computes several parameter inferences with R optimizer (method L-BFGS-B).

Usage

```

flimoptim_R(
  data,
  ndraw,
  sumstats,
  simulatorQ,
  obj = NULL,
  nsim = 10,
  ninfer = 1,
  lower = 0,
  upper = 1,
  Theta0 = (lower + upper)/2,
  randomTheta0 = FALSE,
  maxit = 1000,
  factr = 1e+07,
  pgtol = 0,
  show_trace = FALSE,
  store_quantiles = FALSE,
  par_names = NULL
)

```

Arguments

| | |
|--------------|---|
| data | 1D array containing the observations. |
| ndraw | Integer. Number of random variables to draw for one simulation of the model. |
| sumstats | Summary statistics to measure distance between simulations and data. R function of type <code>sumstats(simulations, data)</code> where <code>simulations</code> : 2D array and <code>data</code> : 1D array. <code>ncol(simulations) = length(data)</code> mandatory. |
| simulatorQ | Simulator of the stochastic process with fixed quantiles (see README). <code>Theta</code> is the parameter set for the simulations and quantiles are drawn in $U(0,1)$. |
| obj | Objective function to minimize. Default : is directly computed from <code>sumstats</code> and <code>simulatorQ</code> . R function of type <code>objective(Theta, quantiles)</code> |
| nsim | Integer. Number of simulations to run for each step of the optimization algorithm. Computation time grows linearly with this number. Default to 10. |
| ninfer | Integer. Number of independent inferences to run. Default to 1. |
| lower | 1D array. Lower bounds for parameters. Same length as <code>upper</code> . |
| upper | 1D array. Upper bounds for parameters. Same length as <code>lower</code> . |
| Theta0 | 1D array. Initial values of the parameters. Default : <code>mean(lower, upper)</code> . |
| randomTheta0 | Boolean. If True, <code>Theta0</code> is randomly drawn between lower and upper bounds. |
| maxit | Integer. Max number of iterations during optimization. Default to 1000. |
| factr | Float. Control parameter for L-BFGS-B method in <code>stats::optim</code> . Default to <code>1e7</code> . |
| pgtol | Float. Control parameter for L-BFGS-B method in <code>stats::optim</code> . Default to 0. |
| show_trace | Boolean. If true, shows standard trace. Default to false. |

store_quantiles Boolean. If true, stores every quantiles used for inference, to reproduce the results.

par_names vector of names for parameters. Default is "par1", ..., "parn".

Value

Object of class flimo_result (list) containing every information about convergence results.

| | |
|------------|-------------------|
| julia_load | <i>julia_load</i> |
|------------|-------------------|

Description

Load needed Julia packages. Run to use Jflimo.

Usage

julia_load()

Value

Boolean. True if load is done correctly

| | |
|-------------|--------------------|
| julia_setup | <i>julia_setup</i> |
|-------------|--------------------|

Description

Checks installation of Julia and install the needed packages. May take little time to run. Only run the first time you use Jflimo.

Usage

julia_setup()

Value

Boolean. True if correct setup, False else.

plot.flimo_result *plot.flimo_result*

Description

Shows the plots for most important inference results. Default only shows normalized boxplots for each inferred parameter.

Usage

```
## S3 method for class 'flimo_result'
plot(
  x,
  y,
  ...,
  hist = FALSE,
  bins = 1 + as.integer(nrow(x$minimizer)^(1/3)),
  par_minimum = FALSE,
  pairwise_par = FALSE,
  boxplot = TRUE,
  par_names = NULL
)
```

Arguments

| | |
|--------------|--|
| x | Object of class flimo_result. |
| y | unused generic argument. |
| ... | optional args for generic method |
| hist | Boolean. If True, plots the histogram of each inferred parameter. Default to false. |
| bins | Integer. Number of bins if hist is True. |
| par_minimum | Boolean. If True, plots each inferred parameter by reached minimum. Default to false. |
| pairwise_par | Boolean. If True, plots each pairs of inferred parameters. Default to false. |
| boxplot | Boolean. If True, plots the boxplots of each inferred parameter scaled by their mean. Default to true. |
| par_names | Vector of names for parameters. Default is "par1", ..., "parn". |

Value

Nothing. Prints the asked ggplot objects.

plot_objective *plot_objective*

Description

Plot of objective = f(theta_index).

Usage

```
plot_objective(
  ndraw,
  nsim,
  data,
  sumstats,
  simulatorQ,
  quantiles = NULL,
  obj = NULL,
  index = NULL,
  other_param = NULL,
  lower = 0,
  upper = 1,
  dim2 = TRUE,
  visualize_min = TRUE,
  plot_legend = TRUE,
  add_to_plot = NULL
)
```

Arguments

| | |
|------------|--|
| ndraw | Integer. Number of random variables to draw for one simulation of the model. |
| nsim | Integer. Number of simulations to run for each step of the optimization algorithm. Computation time grows linearly with this number. Default to 10. |
| data | 1D array containing the observations. |
| sumstats | Function computing the distance between simulations and data of form sumstats(simulations, data) where simulations : 2D array and data : 1D array. ncol(simulations) = length(data) mandatory. |
| simulatorQ | Function of type simulatorQ(Theta, quantiles) where Theta is the parameter set for the simulations and quantiles are drawn in U(0,1). |
| quantiles | 2D array containing values following U(0,1). Row number = number of simulations. Column number = number of random variables to draw in one simulation. |
| obj | objective function of type objective(Theta). Default : directly computed with "sumstats" and "simulatorQ". |
| index | Integer. Index of the moving parameter. |

| | |
|---------------|--|
| other_param | Other parameters of the model. If NULL : assume 1D-model. If numeric : 2D-model, one curve. If 1D-array and dim2 is True (default) : 2D-model, one curve by value in other_param. If 1D-array and dim2 is False or 2D-array : (n>2)D-model, one curve by row in other_param. If your model has n>2 dimensions, you should define other_param as a matrix even if you have only one parameter set to test (with as.matrix(t(vect_param)) where vect_param is a 1D-array). |
| lower | Numeric. Lower value of the plot. |
| upper | Numeric. Upper value of the plot. |
| dim2 | Boolean. True if model is 2-dimensional. |
| visualize_min | Boolean. If True, show explicitly the minimum point. |
| plot_legend | Boolean. If True (default), plots the legend. |
| add_to_plot | ggplot object. If not NULL, will add all curves/points on previous plot instead of creating a new one. Does not change title/labels/limits defined in previous plot. |

Value

ggplot object representing the objective function to be minimized.

Examples

```
data <- rep(100, 5)

sumstats <- function(simulations, data){
  mean_simu <- mean(rowMeans(simulations))
  mean_data <- mean(data)
  (mean_simu-mean_data)^2
}

simulatorQ <- function(Theta, quantiles){
  qpois(quantiles, lambda = Theta)
}

plot_objective(5, 10, data, sumstats, simulatorQ, lower = 0, upper = 200)
```

```
print.flimo_result    print.flimo_result
```

Description

Prints most important information about inference results.

Usage

```
## S3 method for class 'flimo_result'
print(x, ...)
```

Arguments

- x Object of class flimo_result from any mod/method algorithm of the flimo package.
- ... optional args for generic method

Value

String containing most important information about argument of class flimo_result.

summary.flimo_result *summary.flimo_result*

Description

Most important information about inference results.

Usage

```
## S3 method for class 'flimo_result'  
summary(object, ...)
```

Arguments

- object Object of class flimo_result from any mode/method algorithm of the Jflimo package.
- ... optional args for generic method summary

Value

List containing most important information about argument of class flimo_result.

Index

`check_simulator`, 2

`flimobjective`, 3

`flimoptim`, 4

`flimoptim_Julia`, 6

`flimoptim_R`, 8

`julia_load`, 10

`julia_setup`, 10

`plot.flimo_result`, 11

`plot_objective`, 12

`print.flimo_result`, 13

`summary.flimo_result`, 14