Package 'simlandr'

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Type Package

Title Simulation-Based Landscape Construction for Dynamical Systems

Version 0.4.0

Description A toolbox for constructing potential landscapes for dynamical systems using Monte Carlo simulation. The method is based on the potential landscape definition by Wang et al. (2008) <doi:10.1073/pnas.0800579105> (also see Zhou & Li, 2016 <doi:10.1063/1.4943096> for further mathematical discussions) and can be used for a large variety of models.

License GPL (>= 3)

URL https://sciurus365.github.io/simlandr/, https://github.com/Sciurus365/simlandr

BugReports https://github.com/Sciurus365/simlandr/issues

Depends R (>= 4.1.0)

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Contents

`arg_set-class` *Create and modify argument sets, then make an argument grid for batch simulation*

Description

An argument set contains the descriptions of the relevant variables in a batch simulation. Use `new_arg_set()` to create an `arg_set` object, and use `add_arg_ele()` to add an element to the `arg_set`. After adding all elements in the argument set, use `make_arg_grid()` to make an argument grid that can be used directly for running batch simulation.

Usage

```
new_arg_set()

add_arg_ele(arg_set, arg_name, ele_name, start, end, by)

nele(arg_set)
```

```
narg(arg_set)

## S3 method for class 'arg_set'
print(x, detail = FALSE, ...)

make_arg_grid(arg_set)

## S3 method for class 'arg_grid'
print(x, detail = FALSE, ...)
```

Arguments

arg_set	An arg_set object.
arg_name, ele_name	The name of the argument and its element in the simulation function
start, end, by	The data points where you want to test the variables. Passed to seq.
x	An arg_set object
detail	Do you want to print the object details as a full list?
...	Not in use.

Value

new_arg_set() returns an arg_set object.

add_arg_ele() returns an arg_set object.

nele() returns an integer.

narg() returns an integer.

make_arg_gird() returns an arg_grid object.

Functions

- new_arg_set(): Create an arg_set.
- add_arg_ele(): Add an element to an arg_set.
- nele(): The number of elements in an arg_set.
- narg(): The number of arguments in an arg_set.
- print(arg_set): Print an arg_set object.
- make_arg_grid(): Make an argument grid from an argument set.
- print(arg_grid): Print an arg_grid object

See Also

batch_simulation() for running batch simulation and a concrete example.

as.mcmc.list.list *Convert a list of simulation output to a mcmc.list object*

Description

This function can be used to convert a list of simulation output to a mcmc.list object. This may be useful when the output of the simulation is a list of matrices, and you want to perform convergence checks using the functions in the coda package. See `coda::mcmc.list()` for more information, and also see the examples in the documentation of `sim_SDE()`.

Usage

```
## S3 method for class 'list'
as.mcmc.list(x, ...)
```

Arguments

x	A list of simulation output
...	Not used

Value

A mcmc.list object

attach_all_matrices *Attach all matrices in a batch simulation*

Description

Attach all matrices in a batch simulation

Usage

```
attach_all_matrices(bs, backingpath = "bp")
```

Arguments

bs	A `batch_simulation` object.
backingpath	Passed to `bigmemory::as.big.matrix()`.

Value

A `batch_simulation` object with all `hash_big_matrixes` attached.

autolayer.barrier *Get a ggplot2 layer from a barrier object*

Description

This layer can show the saddle point (2d) and the minimal energy path (3d) on the landscape.

Usage

```
## S3 method for class 'barrier'
autolayer(object, path = TRUE, ...)
```

Arguments

object	A barrier object.
path	Show the minimum energy path in the graph?
...	Not in use.

Value

A ggplot2 layer that can be added to an existing landscape plot.

batch_simulation *Perform a batch simulation.*

Description

Perform a batch simulation.

Usage

```
batch_simulation(
  arg_grid,
  sim_fun,
  default_list = list(),
  bigmemory = TRUE,
  ...
)

## S3 method for class 'batch_simulation'
print(x, detail = FALSE, ...)
```

Arguments

arg_grid	An arg_grid object. See make_arg_grid().
sim_fun	The simulation function. See sim_fun_test() for an example.
default_list	A list of default values for sim_fun.
bigmemory	Use hash_big_matrix-class() to store large matrices?
...	Other parameters passed to sim_fun
x	An arg_set object
detail	Do you want to print the object details as a full list?

Value

A batch_simulation object, also a data frame. The first column, var, is a list of ele_list that contains all the variables; the second to the second last columns are the values of the variables; the last column is the output of the simulation function.

Functions

- batch_simulation(): Perform a batch simulation.

Examples

```
batch_arg_set_grad <- new_arg_set()
batch_arg_set_grad <- batch_arg_set_grad %>%
  add_arg_ele(
    arg_name = "parameter", ele_name = "a",
    start = -6, end = -1, by = 1
  )
batch_grid_grad <- make_arg_grid(batch_arg_set_grad)
batch_output_grad <- batch_simulation(batch_grid_grad, sim_fun_grad,
  default_list = list(
    initial = list(x = 0, y = 0),
    parameter = list(a = -4, b = 0, c = 0, sigmasq = 1)
  ),
  length = 1e2,
  seed = 1614,
  bigmemory = FALSE
)
print(batch_output_grad)
```

---

calculate_barrier *Functions for calculating energy barrier from landscapes*

Description

Functions for calculating energy barrier from landscapes

Usage

```
calculate_barrier(l, ...)

## S3 method for class '`2d_landscape`'
calculate_barrier(
  l,
  start_location_value,
  start_r,
  end_location_value,
  end_r,
  base = exp(1),
  ...
)

## S3 method for class '`3d_landscape`'
calculate_barrier(
  l,
  start_location_value,
  start_r,
  end_location_value,
  end_r,
  Umax,
  expand = TRUE,
  omit_unstable = FALSE,
  base = exp(1),
  ...
)

## S3 method for class '`2d_landscape_batch`'
calculate_barrier(
  l,
  bg = NULL,
  start_location_value,
  start_r,
  end_location_value,
  end_r,
  base = exp(1),
  ...
)

## S3 method for class '`3d_landscape_batch`'
calculate_barrier(
  l,
  bg = NULL,
  start_location_value,
  start_r,
  end_location_value,
  end_r,
```

```
  Umax,
  expand = TRUE,
  omit_unstable = FALSE,
  base = exp(1),
  ...
)
```

Arguments

l	A landscape object.
...	Not in use.
start_location_value, end_location_value	The initial position (in value) for searching the start/end point.
start_r, end_r	The search radius (in L1 distance) for the start/end point.
base	The base of the log function.
Umax	The highest possible value of the potential function.
expand	If the values in the range all equal to Umax, expand the range or not?
omit_unstable	If a state is not stable (the "local minimum" overlaps with the saddle point), omit that state or not?
bg	A 2d_barrier_grid or 3d_barrier_grid object if you want to use different parameters for each condition. Otherwise NULL as default.

Value

A barrier object that contains the (batch) barrier calculation result(s).

---

check_conv *Graphical diagnoses to check if the simulation converges*

Description

Compare the distribution of different stages of simulation (for plot_type == "bin" or plot_type = "density"), or show how the percentiles of the distribution evolve over time (for plot_type == cumuplot, see coda::cumuplot() for details). More convergence checking methods for MCMC data are available at the coda package. Be cautious: each convergence checking method has its shortcomings, so do not blindly use any results as the definitive conclusion that a simulation converges or not.

Usage

```
check_conv(output, vars, sample_perc = 0.2, plot_type = "bin")

## S3 method for class 'check_conv'
print(x, ask = TRUE, ...)
```

Arguments

output	A matrix of simulation output, or a multi_init_simulation object generated from multi_init_simulation().
vars	The names of variables to check.
sample_perc	The percentage of data sample for the initial, middle, and final stage of the simulation. Not required if plot_type == "cumuplot".
plot_type	Which type of plots should be generated? ("bin", "density", or "cumuplot" which uses coda::cumuplot())
x	The object.
ask	Ask to press enter to see the next plot?
...	Not in use.

Value

A check_conv object that contains the convergence checking result(for plot_type == "bin" or plot_type = "density"), or draw the cumuplot without a return value (for plot_type == cumuplot).

Methods (by generic)

- print(check_conv): Print a check_conv object.

---

get_dist *Get the probability distribution from a landscape object*

Description

Get the probability distribution from a landscape object

Usage

```
get_dist(l, index = 1)
```

Arguments

l	A landscape project.
index	1 to get the distribution in tidy format; 2 or "raw" to get the raw simulation result (batch_simulation).

Value

A data.frame that contains the distribution in the tidy format or the raw simulation result.

hash_big_matrix-class *Class "hash_big_matrix": big matrix with a md5 hash reference*

Description

hash_big_matrix class is a modified class from bigmemory::big.matrix-class(). Its purpose is to help users operate big matrices within hard disk in a reusable way, so that the large matrices do not consume too much memory, and the matrices can be reused for the next time. Comparing with bigmemory::big.matrix-class(), the major enhancement of hash_big_matrix class is that the backing files are, by default, stored in a permanent place, with the md5 of the object as the file name. With this explicit name, hash_big_matrix objects can be easily reloaded into workspace every time.

Usage

```
as_hash_big_matrix(x, backingpath = "bp", silence = TRUE, ...)

attach_hash_big_matrix(x, backingpath = "bp")
```

Arguments

x	A matrix, vector, or data.frame for bigmemory::as.big.matrix().
backingpath, ...	Passed to bigmemory::as.big.matrix().
silence	Suppress messages?

Functions

- as_hash_big_matrix(): Create a hash_big_matrix object from a matrix.
- attach_hash_big_matrix(): Attach a hash_big_matrix object from the backing file to the workspace.

Slots

md5 The md5 value of the matrix.

address Inherited from big.matrix.

make_2d_matrix *Make a matrix of 2D static landscape plots for one or two parameters*

Description

Make a matrix of 2D static landscape plots for one or two parameters

Usage

```
make_2d_matrix(
  bs,
  x,
  rows = NULL,
  cols,
  lims,
  kde_fun = c("ks", "base"),
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  individual_landscape = TRUE
)
```

Arguments

bs	A batch_simulation object created by [batch_simulation()].
x	The name of the target variable.
rows, cols	The names of the parameters. rows can be left blank if only one parameter is needed.
lims	The limits of the range for the density estimator as c(xl, xu) for 2D landscapes, c(xl, xu, yl, yu) for 3D landscapes, c(xl, xu, yl, yu, zl, zu) for 4D landscapes. If missing, the range of the data extended by 10% for both sides will be used. For landscapes based on multiple simulations, the largest range of all simulations (which means the lowest lower limit and the highest upper limit) will be used by default.
kde_fun	Which kernel estimator to use? Choices: "ks" ks::kde() (default; faster and using less memory); "base" base::density() (only for 2D landscapes); "MASS" MASS::kde2d() (only for 3D landscapes).
n	The number of equally spaced points in each axis, at which the density is to be estimated.
h	A number, or possibly a vector for 3D and 4D landscapes, specifying the smoothing bandwidth to be used. If missing, the default value of the kernel estimator will be used (but bw = "SJ" for base::density()). Note that the definition of bandwidth might be different for different kernel estimators. For landscapes based on multiple simulations, the largest h of all simulations will be used by default.

adjust The multiplier to the bandwidth. The bandwidth used is actually adjust * h. This makes it easy to specify values like "half the default" bandwidth.

Umax The maximum displayed value of potential.

individual_landscape
Make individual landscape for each simulation? Default is TRUE so that it is possible to calculate barriers. Set to FALSE to save time.

Value

A 2d_matrix_landscape object that describes the landscape of the system, including the smoothed distribution and the landscape plot.

---

make_2d_static *Make 2D static landscape plot for a single simulation output*

Description

Make 2D static landscape plot for a single simulation output

Usage

```
make_2d_static(
  output,
  x,
  lims,
  kde_fun = c("ks", "base"),
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  weight_var = NULL
)

make_2d_single(
  output,
  x,
  lims,
  kde_fun = c("ks", "base"),
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  weight_var = NULL
)
```

Arguments

output	A matrix of simulation output, or a mcmc, mcmc.list object (see coda::mcmc()).
x	The name of the target variable.
lims	The limits of the range for the density estimator as c(xl, xu) for 2D landscapes, c(xl, xu, yl, yu) for 3D landscapes, c(xl, xu, yl, yu, zl, zu) for 4D landscapes. If missing, the range of the data extended by 10% for both sides will be used. For landscapes based on multiple simulations, the largest range of all simulations (which means the lowest lower limit and the highest upper limit) will be used by default.
kde_fun	Which kernel estimator to use? Choices: "ks" ks::kde() (default; faster and using less memory); "base" base::density() (only for 2D landscapes); "MASS" MASS::kde2d() (only for 3D landscapes).
n	The number of equally spaced points in each axis, at which the density is to be estimated.
h	A number, or possibly a vector for 3D and 4D landscapes, specifying the smoothing bandwidth to be used. If missing, the default value of the kernel estimator will be used (but bw = "SJ" for base::density()). Note that the definition of bandwidth might be different for different kernel estimators. For landscapes based on multiple simulations, the largest h of all simulations will be used by default.
adjust	The multiplier to the bandwidth. The bandwidth used is actually adjust * h. This makes it easy to specify values like "half the default" bandwidth.
Umax	The maximum displayed value of potential.
weight_var	The name of the weight variable, in case the weight of each observation is different. This may be useful when a weighted MC (e.g., importance sampling) is used. Only effective for kde_fun = "ks".

Value

A 2d_static_landscape object that describes the landscape of the system, including the smooth distribution and the landscape plot.

---

make_3d_animation *Make 3d animations from multiple simulations*

Description

Make 3d animations from multiple simulations

Usage

```
make_3d_animation(
  bs,
  x,
  y,
  fr,
  lims,
  kde_fun = c("ks", "MASS"),
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  individual_landscape = TRUE,
  mat_3d = FALSE
)
```

Arguments

bs	A batch_simulation object created by [batch_simulation()].
x, y	The names of the target variables.
fr	The names of the parameters used to represent frames in the animation.
lims	The limits of the range for the density estimator as c(xl, xu) for 2D landscapes, c(xl, xu, yl, yu) for 3D landscapes, c(xl, xu, yl, yu, zl, zu) for 4D landscapes. If missing, the range of the data extended by 10% for both sides will be used. For landscapes based on multiple simulations, the largest range of all simulations (which means the lowest lower limit and the highest upper limit) will be used by default.
kde_fun	Which kernel estimator to use? Choices: "ks" ks::kde() (default; faster and using less memory); "base" base::density() (only for 2D landscapes); "MASS" MASS::kde2d() (only for 3D landscapes).
n	The number of equally spaced points in each axis, at which the density is to be estimated.
h	A number, or possibly a vector for 3D and 4D landscapes, specifying the smoothing bandwidth to be used. If missing, the default value of the kernel estimator will be used (but bw = "SJ" for base::density()). Note that the definition of bandwidth might be different for different kernel estimators. For landscapes based on multiple simulations, the largest h of all simulations will be used by default.
adjust	The multiplier to the bandwidth. The bandwidth used is actually adjust * h. This makes it easy to specify values like "half the default" bandwidth.
Umax	The maximum displayed value of potential.
individual_landscape	Make individual landscape for each simulation? Default is TRUE so that it is possible to calculate barriers. Set to FALSE to save time.
mat_3d	Also make the matrix by make_3d_matrix()? If so, the matrix can be drawn with plot(<landscape>, 3).

Value

A 3d_animation_landscape object that describes the landscape of the system, including the smoothed distribution and the landscape plot.

---

make_3d_matrix *Make a matrix of 3D static landscape plots for one or two parameters*

Description

Currently only 3D (x, y, color) is supported. Matrices with 3D (x, y, z) plots are not supported.

Usage

```
make_3d_matrix(
  bs,
  x,
  y,
  rows = NULL,
  cols,
  lims,
  kde_fun = c("ks", "MASS"),
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  individual_landscape = TRUE
)
```

Arguments

bs	A batch_simulation object created by [batch_simulation()].
x, y	The names of the target variables.
rows, cols	The names of the parameters. rows can be left blank if only one parameter is needed.
lims	The limits of the range for the density estimator as c(xl, xu) for 2D landscapes, c(xl, xu, yl, yu) for 3D landscapes, c(xl, xu, yl, yu, zl, zu) for 4D landscapes. If missing, the range of the data extended by 10% for both sides will be used. For landscapes based on multiple simulations, the largest range of all simulations (which means the lowest lower limit and the highest upper limit) will be used by default.
kde_fun	Which kernel estimator to use? Choices: "ks" ks::kde() (default; faster and using less memory); "base" base::density() (only for 2D landscapes); "MASS" MASS::kde2d() (only for 3D landscapes).
n	The number of equally spaced points in each axis, at which the density is to be estimated.

h — A number, or possibly a vector for 3D and 4D landscapes, specifying the smoothing bandwidth to be used. If missing, the default value of the kernel estimator will be used (but bw = "SJ" for base::density()). Note that the definition of bandwidth might be different for different kernel estimators. For landscapes based on multiple simulations, the largest h of all simulations will be used by default.

adjust — The multiplier to the bandwidth. The bandwidth used is actually adjust * h. This makes it easy to specify values like "half the default" bandwidth.

Umax — The maximum displayed value of potential.

individual_landscape — Make individual landscape for each simulation? Default is TRUE so that it is possible to calculate barriers. Set to FALSE to save time.

Value

A 3d_matrix_landscape object that describes the landscape of the system, including the smoothed distribution and the landscape plot.

---

make_3d_static *Make 3D static landscape plots from simulation output*

Description

Make 3D static landscape plots from simulation output

Usage

```
make_3d_static(
  output,
  x,
  y,
  lims,
  kde_fun = c("ks", "MASS"),
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  weight_var = NULL
)

make_3d_single(
  output,
  x,
  y,
  lims,
  kde_fun = c("ks", "MASS"),
```

```
  n = 200,
  h,
  adjust = 1,
  Umax = 5,
  weight_var = NULL
)
```

Arguments

output	A matrix of simulation output, or a mcmc, mcmc.list object (see coda::mcmc()).
x, y	The names of the target variables.
lims	The limits of the range for the density estimator as c(xl, xu) for 2D landscapes, c(xl, xu, yl, yu) for 3D landscapes, c(xl, xu, yl, yu, zl, zu) for 4D landscapes. If missing, the range of the data extended by 10% for both sides will be used. For landscapes based on multiple simulations, the largest range of all simulations (which means the lowest lower limit and the highest upper limit) will be used by default.
kde_fun	Which kernel estimator to use? Choices: "ks" ks::kde() (default; faster and using less memory); "base" base::density() (only for 2D landscapes); "MASS" MASS::kde2d() (only for 3D landscapes).
n	The number of equally spaced points in each axis, at which the density is to be estimated.
h	A number, or possibly a vector for 3D and 4D landscapes, specifying the smoothing bandwidth to be used. If missing, the default value of the kernel estimator will be used (but bw = "SJ" for base::density()). Note that the definition of bandwidth might be different for different kernel estimators. For landscapes based on multiple simulations, the largest h of all simulations will be used by default.
adjust	The multiplier to the bandwidth. The bandwidth used is actually adjust * h. This makes it easy to specify values like "half the default" bandwidth.
Umax	The maximum displayed value of potential.
weight_var	The name of the weight variable, in case the weight of each observation is different. This may be useful when a weighted MC (e.g., importance sampling) is used. Only effective for kde_fun = "ks".

Value

A 3d_static_landscape object that describes the landscape of the system, including the smooth distribution and the landscape plot.

`make_4d_static` *Make 4D static space-color plots from simulation output*

Description

Make 4D static space-color plots from simulation output

Usage

```
make_4d_static(
  output,
  x,
  y,
  z,
  lims,
  kde_fun = "ks",
  n = 50,
  h,
  adjust = 1,
  Umax = 5,
  weight_var = NULL
)

make_4d_single(
  output,
  x,
  y,
  z,
  lims,
  kde_fun = "ks",
  n = 50,
  h,
  adjust = 1,
  Umax = 5,
  weight_var = NULL
)
```

Arguments

`output`	A matrix of simulation output, or a `mcmc`, `mcmc.list` object (see `coda::mcmc()`).
`x, y, z`	The names of the target variables.
`lims`	The limits of the range for the density estimator as `c(xl, xu)` for 2D landscapes, `c(xl, xu, yl, yu)` for 3D landscapes, `c(xl, xu, yl, yu, zl, zu)` for 4D landscapes. If missing, the range of the data extended by 10% for both sides will be used. For landscapes based on multiple simulations, the largest range of all simulations (which means the lowest lower limit and the highest upper limit) will be used by default.

kde_fun	Which kernel estimator to use? Choices: "ks" ks::kde() (default; faster and using less memory); "base" base::density() (only for 2D landscapes); "MASS" MASS::kde2d() (only for 3D landscapes).
n	The number of equally spaced points in each axis, at which the density is to be estimated.
h	A number, or possibly a vector for 3D and 4D landscapes, specifying the smoothing bandwidth to be used. If missing, the default value of the kernel estimator will be used (but bw = "SJ" for base::density()). Note that the definition of bandwidth might be different for different kernel estimators. For landscapes based on multiple simulations, the largest h of all simulations will be used by default.
adjust	The multiplier to the bandwidth. The bandwidth used is actually adjust * h. This makes it easy to specify values like "half the default" bandwidth.
Umax	The maximum displayed value of potential.
weight_var	The name of the weight variable, in case the weight of each observation is different. This may be useful when a weighted MC (e.g., importance sampling) is used. Only effective for kde_fun = "ks".

Value

A 4d_static_landscape object that describes the landscape of the system, including the smoothed distribution and the landscape plot.

---

make_barrier_grid_2d *Make a grid for calculating barriers for 2d landscapes*

Description

Make a grid for calculating barriers for 2d landscapes

Usage

```
make_barrier_grid_2d(
  ag,
  start_location_value,
  start_r,
  end_location_value,
  end_r,
  df = NULL,
  print_template = FALSE
)
```

Arguments

ag	An arg_grid object.
start_location_value, start_r, end_location_value, end_r	Default values for finding local minimum. See calculate_barrier().
df	A data frame for the variables. Use print_template = TRUE to get a template.
print_template	Print a template for df.

Value

A barrier_grid_2d object that specifies the condition for each barrier calculation.

---

make_barrier_grid_3d *Make a grid for calculating barriers for 3d landscapes*

Description

Make a grid for calculating barriers for 3d landscapes

Usage

```
make_barrier_grid_3d(
  ag,
  start_location_value,
  start_r,
  end_location_value,
  end_r,
  df = NULL,
  print_template = FALSE
)
```

Arguments

ag	An arg_grid object.
start_location_value, start_r, end_location_value, end_r	Default values for finding local minimum. See calculate_barrier().
df	A data frame for the variables. Use print_template = TRUE to get a template.
print_template	Print a template for df.

Value

A barrier_grid_3d object that specifies the condition for each barrier calculation.

multi_init_simulation *Simulate multiple 1-3D Markovian Stochastic Differential Equations*

Description

Simulate multiple Monte Carlo simulations of 1-3D Markovian Stochastic Differential Equations from a grid or random sample of initial values. Parallel processing is supported. To register a parallel backend, use `future::plan()`. For example, `future::plan(future::multisession)`. For more information, see `future::plan()`. Functions imported from other programming languages, such as C++ or Python functions, may not work in parallel processing. If you are uncertain whether there are unknown stable states of the system that are difficult to reach, it is recommended to start with running a large number (i.e., increasing `R`) of short simulations to see if the system reaches to the known stable states.

Usage

```
multi_init_simulation(
  sim_fun,
  R = 10,
  range_x0,
  sample_mode = c("grid", "random"),
  ...,
  .furrr_options = list(.options = furrr::furrr_options(seed = TRUE)),
  return_object = c("mcmc.list", "raw")
)
```

Arguments

`sim_fun`	The simulation function to use. It should accept an argument `x0` for the initial values. Other arguments can be passed through `...`.
`R`	The number of initial values to sample. If `sample_mode` is "grid", this will be the number of initial values in each dimension. If `sample_mode` is "random", this will be the total number of initial values.
`range_x0`	The range of initial values to sample in a vector of length 2 for each dimension (i.e., `c(<x0_minimum>, <x0_maximum>, <y0_minimum>, <y0_maximum>, <z0_minimum>, <z0_maximu`
`sample_mode`	The mode of sampling initial values. Either "grid" or "random". If "grid", the initial values will be sampled from a grid. If "random", the initial values will be sampled randomly.
`...`	Additional arguments passed to `sim_fun`.
`.furrr_options`	A list of options to be passed to `furrr::future_pmap()`.
`return_object`	The type of object to return. Either "mcmc.list" or "raw". If "mcmc.list", a list of mcmc objects will be returned. If "raw", a tibble of initial values and raw simulation results will be returned.

Value

A list of mcmc objects or a tibble of initial values and raw simulation results, depending on the value of `return_object`.

Examples

```
# Adapted from the example in the Sim.DiffProc package

set.seed(1234, kind = "L'Ecuyer-CMRG")
mu <- 4
sigma <- 0.1
fx <- expression(y, (mu * (1 - x^2) * y - x))
gx <- expression(0, 2 * sigma)

multiple_mod2d <- multi_init_simulation(sim_SDE, range_x0 = c(-3, 3, -10, 10),
R = 3, sample_mode = "grid", drift = fx, diffusion = gx,
N = 1000, Dt = 0.01, type = "str", method = "rk1",
keep_full = FALSE, M = 2)

# The output is a mcmc.list object. You can use the functions
# in the coda package to modify it and perform convergence check,
# for example,

library(coda)
plot(multiple_mod2d)
window(multiple_mod2d, start = 500)
effectiveSize(multiple_mod2d)
```

---

plot.landscape *Make plots from landscape objects*

Description

Make plots from landscape objects

Usage

```
## S3 method for class 'landscape'
plot(x, index = 1, ...)
```

Arguments

`x`	A landscape object
`index`	Default is 1. For some landscape objects, there is a second plot (usually 2d heatmaps for 3d landscapes) or a third plot (usually 3d matrices for 3d animations). Use `index = 2` to plot that one.
`...`	Not in use.

Value

The plot.

`save_landscape` *Save landscape plots*

Description

Save landscape plots

Usage

```
save_landscape(l, path = NULL, selfcontained = FALSE, ...)
```

Arguments

`l`	A landscape object
`path`	The path to save the output. Default: "/pics/x_y.html".
`selfcontained`	For 'plotly' plots, save the output as a self-contained html file? Default: FALSE.
`...`	Other parameters passed to `htmlwidgets::saveWidget()` or `ggplot2::ggsave()`

Value

The function saves the plot to a specific path. It does not have a return value.

`sim_fun_grad` *A simple gradient simulation function for testing*

Description

This is a toy stochastic gradient system which can have bistability in some conditions. Model specification:

$$U = x^4 + y^4 + axy + bx + cy$$
$$dx/dt = -\partial U/\partial x + \sigma dW/dt = -4x^3 - ay - b + \sigma dW/dt$$
$$dy/dt = -\partial U/\partial y + \sigma dW/dt = -4y^3 - ax - c + \sigma dW/dt$$

Usage

```
sim_fun_grad(
  initial = list(x = 0, y = 0),
  parameter = list(a = -4, b = 0, c = 0, sigmasq = 1),
  length = 1e+05,
  stepsize = 0.01,
  seed = NULL
)
```

Arguments

initial, parameter	Two sets of parameters. initial contains the initial value of x and y; parameter contains a, b, c, which control the shape of the potential landscape, and sigmasq, which is the square of σ and controls the amplitude of noise.
length	The length of simulation.
stepsize	The step size used in the Euler method.
seed	The initial seed that will be passed to set.seed() function.

Value

A matrix of simulation results.

See Also

sim_fun_nongrad() and batch_simulation().

---

sim_fun_nongrad *A simple non-gradient simulation function for testing*

Description

This is a toy stochastic non-gradient system which can have multistability in some conditions. Model specification:

Usage

```
sim_fun_nongrad(
  initial = list(x1 = 0, x2 = 0, a = 1),
 parameter = list(b = 1, k = 1, S = 0.5, n = 4, lambda = 0.01, sigmasq1 = 8, sigmasq2 =
    8, sigmasq3 = 2),
  constrain_a = TRUE,
  amin = -0.3,
  amax = 1.8,
  length = 1e+05,
  stepsize = 0.01,
  seed = NULL,
  progress = TRUE
)
```

Arguments

initial, parameter	Two sets of parameters. initial contains the initial value of x1, x2, and a; parameter contains b,k,S,n,lambda, which control the model dynamics, and sigmasq1,sigmasq2,sigmasq3, which are the squares of $\sigma_1, \sigma_2, \sigma_3$ and controls the amplitude of noise.

constrain_a	Should the value of a be constrained? (TRUE by default).
amin, amax	If constrain_a, the minimum and maximum values of a.
length	The length of simulation.
stepsize	The step size used in the Euler method.
seed	The initial seed that will be passed to set.seed() function.
progress	Show progress bar of the simulation?

Details

$$\frac{dx_1}{dt} = \frac{ax_1^n}{S^n + x_1^n} + \frac{bS^n}{S^n + x_2^n} - kx_1 + \sigma_1 dW_1/dt$$
$$\frac{dx_2}{dt} = \frac{ax_2^n}{S^n + x_2^n} + \frac{bS^n}{S^n + x_1^n} - kx_2 + \sigma_2 dW_2/dt$$
$$\frac{da}{dt} = -\lambda a + \sigma_3 dW_3/dt$$

Value

A matrix of simulation results.

References

Wang, J., Zhang, K., Xu, L., & Wang, E. (2011). Quantifying the Waddington landscape and biological paths for development and differentiation. Proceedings of the National Academy of Sciences, 108(20), 8257-8262. doi:10.1073/pnas.1017017108

See Also

sim_fun_grad() and batch_simulation().

---

sim_fun_test *A simple simulation function for testing*

Description

A simple simulation function for testing

Usage

```
sim_fun_test(arg1, arg2, length = 1000)
```

Arguments

arg1, arg2	Two parameters. arg1 contains ele1; arg2 contains ele2 and ele3.
length	The length of simulation.

Value

A matrix of simulation results.

See Also

`sim_fun_grad()` and `sim_fun_nongrad()` for more realistic examples.

`sim_SDE` *Simulate 1-3D Markovian Stochastic Differential Equations*

Description

A wrapper to the simulation utilities provided by the **Sim.DiffProc** package. You may skip this step and write your own simulation function for more customized simulation.

Usage

```
sim_SDE(
  N = 1000,
  M = 1,
  x0,
  t0 = 0,
  T = 1,
  Dt = rlang::missing_arg(),
  drift,
  diffusion,
  corr = NULL,
  alpha = 0.5,
  mu = 0.5,
  type = "ito",
  method = "euler",
  keep_full = TRUE
)
```

Arguments

`N`	The number of time steps.
`M`	The number of simulations.
`x0`	The initial values of the SDE. The number of values determine the dimension of the SDE.
`t0`	initial time.
`T`	terminal time.
`Dt`	time step. If missing, default will be (T - t0) / N.
`drift`	An expression of the drift function. The number of expressions determine the dimension of the SDE. Should be the function of `t`, `x`, `y` and `z` (`y` and `z` are only included for 2D or 3D cases).

diffusion	An expression of the diffusion function. The number of expressions determine the dimension of the SDE. Should be the function of t, x, y and z (y and z are only included for 2D or 3D cases).
corr	The correlations between the Brownian motions. Only used for 2D or 3D cases. Must be a real symmetric positive-definite matrix of size 2x2 or 3x3. If NULL, the default is the identity matrix.
alpha, mu	weight of the predictor-corrector scheme; the default alpha = 0.5 and mu = 0.5.
type	if type="ito" simulation sde of Itô type, else type="str" simulation sde of Stratonovich type; the default type="ito".
method	numerical methods of simulation, the default method = "euler".
keep_full	Whether to keep the full snssde1d/snssde2d/snssde3d object. If TRUE, the full object will be returned. If FALSE, only the simulated values will be returned as a matrix or a list of matrices (when M >= 2).

Value

Depending on the value of keep_full, the output will be a list of snssde1d, snssde2d or snssde3d objects, or a matrix or a list of matrices of the simulated values.

Examples

```
# From the Sim.DiffProc package

set.seed(1234, kind = "L'Ecuyer-CMRG")
mu <- 4
sigma <- 0.1
fx <- expression(y, (mu * (1 - x^2) * y - x))
gx <- expression(0, 2 * sigma)
mod2d <- sim_SDE(drift = fx, diffusion = gx, N = 1000,
Dt = 0.01, x0 = c(0, 0), type = "str", method = "rk1",
M = 2, keep_full = FALSE)

print(as.mcmc.list(mod2d))
```

---

summary.barrier *Summarize the barrier height from a* barrier *object*

Description

Summarize the barrier height from a barrier object

Usage

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

Arguments

`object`	A `barrier` object.
`...`	Not in use.

Value

A vector (for a single barrier calculation result) or a `data.frame` (for batch barrier calculation results) that contains the barrier heights on the landscape.

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