Package: mcstate (via r-universe)

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Title Monte Carlo Methods for State Space Models

Version 0.9.22

Description Implements Monte Carlo methods for state-space models such as 'SIR' models in epidemiology. Particle MCMC (pmcmc) and SMC2 methods are planned. This package is particularly designed to work with odin/dust models, but we will see how general it becomes.

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Language en-GB

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BugReports https://github.com/mrc-ide/mcstate/issues

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Contents

`adaptive_proposal_control`

Adaptive proposal control

Description

Control for adaptive proposals, used in pmcmc_control for deterministic models.

Usage

```
adaptive_proposal_control(
  initial_vcv_weight = 1000,
  initial_scaling = 1,
  initial_scaling_weight = NULL,
  min_scaling = 0,
  scaling_increment = NULL,
  log_scaling_update = TRUE,
  acceptance_target = 0.234,
  forget_rate = 0.2,
  forget_end = Inf,
  adapt_end = Inf,
  pre_diminish = 0
)
```

Arguments

`initial_vcv_weight`
: Weight of the initial variance-covariance matrix used to build the proposal of the random-walk. Higher values translate into higher confidence of the initial variance-covariance matrix and means that update from additional samples will be slower.

`initial_scaling`
: The initial scaling of the variance covariance matrix to be used to generate the multivariate normal proposal for the random-walk Metropolis-Hastings algorithm. To generate the proposal matrix, the weighted variance covariance matrix is multiplied by the scaling parameter squared times 2.38^2 / n_pars (where n_pars is the number of fitted parameters). Thus, in a Gaussian target parameter space, the optimal scaling will be around 1.

`initial_scaling_weight`
: The initial weight used in the scaling update. The scaling weight will increase after the first `pre_diminish` iterations, and as the scaling weight increases the adaptation of the scaling diminishes. If `NULL` (the default) the value is 5 / (acceptance_target * (1 - acceptance_target)).

`min_scaling`
: The minimum scaling of the variance covariance matrix to be used to generate the multivariate normal proposal for the random-walk Metropolis-Hastings algorithm.

`scaling_increment`
: The scaling increment which is added or subtracted to the scaling factor of the variance-covariance after each adaptive step. If `NULL` (the default) then an optimal value will be calculated.

`log_scaling_update`
: Logical, whether or not changes to the scaling parameter are made on the log-scale.

`acceptance_target`
: The target for the fraction of proposals that should be accepted (optimally) for the adaptive part of the mixture model.

`forget_rate` The rate of forgetting early parameter sets from the empirical variance-covariance matrix in the MCMC chains. For example, `forget_rate = 0.2` (the default) means that once in every 5th iterations we remove the earliest parameter set included, so would remove the 1st parameter set on the 5th update, the 2nd on the 10th update, and so on. Setting `forget_rate = 0` means early parameter sets are never forgotten.

`forget_end` The final iteration at which early parameter sets can be forgotten. Setting `forget_rate = Inf` (the default) means that the forgetting mechanism continues throughout the chains. Forgetting early parameter sets becomes less useful once the chains have settled into the posterior mode, so this parameter might be set as an estimate of how long that would take.

`adapt_end` The final iteration at which we can adapt the multivariate normal proposal. Thereafter the empirical variance-covariance matrix, its scaling and its weight remain fixed. This allows the adaptation to be switched off at a certain point to help ensure convergence of the chain.

`pre_diminish` The number of updates before adaptation of the scaling parameter starts to diminish. Setting `pre_diminish = 0` means there is diminishing adaptation of the scaling parameter from the offset, while `pre_diminish = Inf` would mean there is never diminishing adaptation. Diminishing adaptation should help the scaling parameter to converge better, but while the chains find the location and scale of the posterior mode it might be useful to explore with it switched off.

Details

Efficient exploration of the parameter space during an MCMC might be difficult when the target distribution is of high dimensionality, especially if the target probability distribution present a high degree of correlation. Adaptive schemes are used to "learn" on the fly the correlation structure by updating the proposal distribution by recalculating the empirical variance-covariance matrix and rescale it at each adaptive step of the MCMC.

Our implementation of an adaptive MCMC algorithm is based on an adaptation of the "accelerated shaping" algorithm in Spencer (2021). The algorithm is based on a random-walk Metropolis-Hasting algorithm where the proposal is a multi-variate Normal distribution centered on the current point.

Spencer SEF (2021) Accelerating adaptation in the adaptive Metropolis–Hastings random walk algorithm. Australian & New Zealand Journal of Statistics 63:468-484.

`array_bind` *Bind arrays*

Description

Bind a number of arrays, usually by their last dimension. This is useful for binding together the sorts of arrays produced by dust and mcstate's simulation functions.

Usage

```
array_bind(..., arrays = list(...), dimension = NULL)
```

Arguments

`...`	Any number of arrays. All dimensions must the the same, except for the dimension being bound on which may vary.
`arrays`	As an alternative to using `...` you can provide a list directly. This is often nicer to program with.
`dimension`	The dimension to bind on; by default `NULL` means the last dimension.

Value

A single array object

Examples

```
# Consider two matricies; this is equivalent to rbind and is
# pretty trivial
m1 <- matrix(1, 4, 5)
m2 <- matrix(2, 4, 2)
mcstate::array_bind(m1, m2)

# For a 4d array though it's less obvious
a1 <- array(1, c(2, 3, 4, 5))
a2 <- array(2, c(2, 3, 4, 1))
a3 <- array(3, c(2, 3, 4, 3))
dim(mcstate::array_bind(a1, a2, a3))
```

`array_drop` *Drop specific array dimensions*

Description

Drop specific array dimensions that are equal to 1. This a more explicit, safer version of drop, which requires you indicate which dimensions will be dropped and errors if dimensions can't be dropped.

Usage

```
array_drop(x, i)
```

Arguments

`x`	An array
`i`	Index or indices of dimensions to remove

Value

An array

Examples

```
# Suppose we have an array with a redundant 2nd dimension
m <- array(1:25, c(5, 1, 5))

# commonly we might drop this with
drop(m)

# in this case, array_drop is the same:
mcstate::array_drop(m, 2)

# However, suppose that our matrix had, in this case, a first
# dimension that was also 1 but we did not want to drop it:
m2 <- m[1, , , drop = FALSE]

# Here, drop(m2) returns just a vector, discarding our first dimension
drop(m2)

# However, array_drop will preserve that dimension
mcstate::array_drop(m2, 2)
```

---

array_flatten *Flatten array dimensions*

Description

Flatten array dimensions into a single dimension. This takes a multidimensional array and converts some dimensions of it into a vector. Use this to drop out "middle" dimensions of a structured array. This is conceptually the inverse of array_reshape

Usage

```
array_flatten(x, i)
```

Arguments

x	An array
i	An integer vector of dimensions to flatten

Value

A new array with at one or more dimensions removed

See Also

array_flatten which adds structure

Examples

```
x <- array(1:12, c(2, 3, 4))
mcstate::array_flatten(x, 2:3)

# array_flatten and array_reshape are each others' conceptual
# opposites:
y <- mcstate::array_flatten(x, 2:3)
identical(mcstate::array_reshape(y, 2, c(3, 4)), x)
```

`array_reshape` *Rehape an array dimension*

Description

Reshape one dimension of a multidimensional array. Use this to say that some dimension (say with length 20) actually represents a number of other dimensions (e.g., 2 x 10 or 2 x 2 x 5). This might be the case if you've been doing a simulation with a large number of parameter sets that are pooled over some other grouping factors (e.g., in a sensitivity analysis)

Usage

```
array_reshape(x, i, d)
```

Arguments

`x`	An array
`i`	The index of the dimension to expand
`d`	The new dimensions for data in the i'th dimension of x

Value

A multidimensional array

See Also

array_flatten which undoes this operation

Examples

```
# Suppose we had a 4 x 6 array of data:
m <- matrix(1:24, 4, 6)

# And suppose that the second dimension really represented a 2 x 3
# matrix; so that looking at one copy of the 2nd dimension we see
m[1, ]

# But instead we might want to see
res <- mcstate::array_reshape(m, 2, c(2, 3))
res[1, , ]
```

`if2` *Run iterated filtering (IF2 algorithm)*

Description

Create an IF2 object for running and interacting with an IF2 inference.

Usage

```
if2(pars, filter, control)

if2_sample(obj, n_particles)
```

Arguments

`pars`	An if2_parameters object, describing the parameters that will be varied in the simulation, and the method of transformation into model parameters.
`filter`	A particle_filter object. We don't use the particle filter directly (except for sampling with `mcstate::if2_sample`) but this shares so much validation that it's convenient. Be sure to set things like the seed and number of threads here if you want to use anything other than the default.
`control`	An `if2_control()` object
`obj`	An object of class `if2_fit`, returned by `mcstate::if2()`
`n_particles`	The number of particles to simulate, for each IF2 parameter set

Details

See: Ionides EL, Nguyen D, Atchadé Y, Stoev S, King AA (2015). "Inference for Dynamic and Latent Variable Models via Iterated, Perturbed Bayes Maps." PNAS, 112(3), 719–724. https://doi.org/10.1073/pnas.1410597112

Value

An object of class `if2_fit`, which contains the sampled parameters (over time) and their log-likelihoods

Examples

```
# A basic SIR model used in the particle filter example
gen <- dust::dust_example("sir")

# Some data that we will fit to, using 1 particle:
sir <- gen$new(pars = list(), time = 0, n_particles = 1)
dt <- 1 / 4
day <- seq(1, 100)
incidence <- rep(NA, length(day))
true_history <- array(NA_real_, c(5, 1, 101))
true_history[, 1, 1] <- sir$state()
```

```
for (i in day) {
  state_start <- sir$state()
  sir$run(i / dt)
  state_end <- sir$state()
  true_history[, 1, i + 1] <- state_end
  # Reduction in S
  incidence[i] <- state_start[1, 1] - state_end[1, 1]
}

# Convert this into our required format:
data_raw <- data.frame(day = day, incidence = incidence)
data <- particle_filter_data(data_raw, "day", 4, 0)

# A comparison function
compare <- function(state, observed, pars = NULL) {
  if (is.null(pars$exp_noise)) {
    exp_noise <- 1e6
  } else {
    exp_noise <- pars$exp_noise
  }
  incidence_modelled <- state[1,]
  incidence_observed <- observed$incidence
  lambda <- incidence_modelled +
    rexp(length(incidence_modelled), exp_noise)
  dpois(incidence_observed, lambda, log = TRUE)
}

# Range and initial values for model parameters
pars <- mcstate::if2_parameters$new(
  list(mcstate::if2_parameter("beta", 0.15, min = 0, max = 1),
       mcstate::if2_parameter("gamma", 0.05, min = 0, max = 1)))

# Set up of IF2 algorithm (the iterations and n_par_sets should be
# increased here for any real use)
control <- mcstate::if2_control(
  pars_sd = list("beta" = 0.02, "gamma" = 0.02),
  iterations = 10,
  n_par_sets = 40,
  cooling_target = 0.5,
  progress = interactive())

# Create a particle filter object
filter <- mcstate::particle_filter$new(data, gen, 1L, compare)

# Then run the IF2
res <- mcstate::if2(pars, filter, control)

# Get log-likelihood estimates from running a particle filter at
# each final parameter estimate
ll_samples <- mcstate::if2_sample(res, 20)
```

if2_control *Control for IF2*

Description

Control for `if2()`. This function constructs a list of options and does some basic validation. Do not manually change the values in this object. Do not refer to any argument by position as the order of the arguments may change in future.

Usage

```
if2_control(pars_sd, iterations, n_par_sets, cooling_target, progress = TRUE)
```

Arguments

`pars_sd`	The initial standard deviation of parameter walks.
`iterations`	The number of IF2 iterations to run, across which the cooling is performed
`n_par_sets`	The number of parameter sets to walk (c.f. the population size)
`cooling_target`	A factor < 1 multiplying pars_sd, which will be reached by the end of the iterations, and approached geometrically
`progress`	Logical, indicating if a progress bar should be displayed, using `progress::progress_bar`.

Value

An `if2_control` object, which should not be modified once created. Pass this into `if2()`

Examples

```
mcstate::if2_control(list(beta = 0.2, gamma = 0.2), 100, 1000, 0.5)
```

if2_parameter *Describe single IF2 parameter*

Description

Describe a single parameter for use within IF2. Note that the name is not set here, but will end up being naturally defined when used with `if2_parameters`, which collects these together for use with `if2()`.

Usage

```
if2_parameter(
  name,
  initial,
  min = -Inf,
  max = Inf,
  discrete,
  integer = FALSE,
  prior = NULL
)
```

Arguments

`name`	Name for the parameter (a string)
`initial`	Initial value of the parameter
`min`	Optional minimum value for the parameter (otherwise `-Inf`). If given, then `initial` must be at least this value.
`max`	Optional max value for the parameter (otherwise `Inf`). If given, then `initial` must be at most this value.
`discrete`	Deprecated; use `integer` instead.
`integer`	Logical, indicating if this parameter is integer. If `TRUE` then the parameter will be rounded after a new parameter is proposed.
`prior`	A prior function (if not given an improper flat prior is used - be careful!). It must be a function that takes a single argument, being the value of this parameter. If given, then `prior(initial)` must evaluate to a finite value.

Examples

```
mcstate::if2_parameter("a", 0.1)
```

`if2_parameters` *if2_parameters*

Description

Construct parameters for use with `if2()`. This creates a utility object that is used internally to work with parameters. Most users only need to construct this object, but see the examples for how it can be used.

Methods

Public methods:

- `if2_parameters$new()`
- `if2_parameters$initial()`

- if2_parameters$walk_initialise()
- if2_parameters$walk()
- if2_parameters$names()
- if2_parameters$summary()
- if2_parameters$prior()
- if2_parameters$model()

Method `new()`**:** Create the if2_parameters object

Usage:

```
if2_parameters$new(parameters, transform = NULL)
```

Arguments:

`parameters` A `list` of `if2_parameter` objects, each of which describe a single parameter in your model. If `parameters` is named, then these names must match the `$name` element of each parameter is used (this is verified).

`transform` An optional transformation function to apply to your parameter vector immediately before passing it to the model function. If not given, then as.list is used, as dust models require this. However, if you need to generate derived parameters from those being actively sampled you can do arbitrary transformations here.

Method `initial()`**:** Return the initial parameter values as a named numeric vector

Usage:

```
if2_parameters$initial()
```

Method `walk_initialise()`**:** Set up a parameter walk

Usage:

```
if2_parameters$walk_initialise(n_par_sets, pars_sd)
```

Arguments:

`n_par_sets` An integer number of parameter sets, which defines the size of the population being peturbed.

`pars_sd` A vector of standard deviations for the walk of each parameter

Method `walk()`**:** Propose a new parameter matrix given a current matrix and walk standard deviation vector.

Usage:

```
if2_parameters$walk(pars, pars_sd)
```

Arguments:

`pars` A parameter matrix, from this function or `$walk_initialise()`

`pars_sd` A vector of standard deviations for the walk of each parameter

Method `names()`**:** Return the names of the parameters

Usage:

```
if2_parameters$names()
```

Method `summary()`**:** Return a `data.frame` with information about parameters (name, min, max, and integer).

Usage:

```
if2_parameters$summary()
```

Method `prior()`**:** Compute the prior for a parameter vector

Usage:

```
if2_parameters$prior(pars)
```

Arguments:

`pars` a parameter matrix from `$walk()`

Method `model()`**:** Apply the model transformation function to a parameter vector. Output is a list for lists, suitable for use with a dust object with `pars_multi = TRUE`

Usage:

```
if2_parameters$model(pars)
```

Arguments:

`pars` a parameter matrix from `$walk()`

Examples

```
# Construct an object with two parameters:
pars <- mcstate::if2_parameters$new(
  list(mcstate::if2_parameter("a", 0.1, min = 0, max = 1,
                              prior = function(a) log(a)),
       mcstate::if2_parameter("b", 0, prior = dnorm)))

# Initial parameters
pars$initial()

# Create the initial parameter set
n_par_sets <- 5
pars_sd <- list("a" = 0.02, "b" = 0.02)
p_mat <- pars$walk_initialise(n_par_sets, pars_sd)
p_mat

# Propose a new parameter set
p_mat <- pars$walk(p_mat, pars_sd)
p_mat

# Information about parameters:
pars$names()
pars$summary()

# Compute prior
pars$prior(p_mat)

# Transform data for your model
pars$model(p_mat)
```

multistage_epoch *Multistage filter epoch*

Description

Describe an epoch within a multistage_parameters object

Usage

```
multistage_epoch(start, pars = NULL, transform_state = NULL)
```

Arguments

start	The start time, in units of time in your data set. These must correspond to time points with data. The model will complete the step to this time point, then change parameters, then continue (so start represents the time point we move from with these parameters)
pars	Optional parameter object, replacing the model parameters at this point. If NULL then the model parameters are not changed, and it is assumed that you will be changing model state via transform_state.
transform_state	Optional parameter transformation function. This could be used in two cases (1) arbitrary change to the model state (e.g., a one-off movement of state within particles at a given time point that would be otherwise awkward to code directly in your model), or (2) where you have provided pars and these imply a different model state size. In this case you *must* provide transform_state to fill in new model state, move things around, or delete model state depending on how the state has changed. This function will be passed three arguments: (1) the current model state, (2) the result of the $info() method from the model used to this point, (3) the result of the $info() method for the new model that was created with pars which will be run from this point. Future versions of this interface may allow passing the parameters in too.

multistage_parameters *Multistage filter parameters*

Description

Construct parameters for a multi-stage particle filter.

Usage

```
multistage_parameters(pars, epochs)
```

Arguments

pars	The parameters covering the period up to the first change in epoch.
epochs	A list of multistage_epoch objects corresponding to a new paramter regime starting at a new time point.

Value

An object of class multistage_parameters, suitable to pass through to the run method of particle_filter

---

particle_deterministic

Deterministic particle likelihood

Description

Create a deterministic version of the particle_filter object, which runs a single particle deterministically.

Public fields

model The dust model generator being simulated (cannot be re-bound)

has_multiple_parameters Logical, indicating if the deterministic particle requires multiple parameter sets in a list as inputs, and if it it will produce a vector of likelihoods the same length (read only). The parameter sets may or may not use the same data (see has_multiple_data).

has_multiple_data Logical, indicating if the deterministic particle simultaneously calculates the likelihood for multiple parameter sets (read only). If TRUE, has_multiple_parameters will always be TRUE.

n_parameters The number of parameter sets used by this deterministic particle (read only). The returned vector of likelihoods will be this length, and if has_multiple_parameters is FALSE this will be 1.

n_data The number of data sets used by this deterministic particle (read only). This will either be 1 or the same value as n_parameters.

Methods

Public methods:

- particle_deterministic$new()
- particle_deterministic$run()
- particle_deterministic$run_begin()
- particle_deterministic$state()
- particle_deterministic$history()
- particle_deterministic$restart_state()
- particle_deterministic$inputs()
- particle_deterministic$set_n_threads()

Method `new()`**:** Create the particle filter

Usage:

```
particle_deterministic$new(
  data,
  model,
  compare,
  index = NULL,
  initial = NULL,
  constant_log_likelihood = NULL,
  n_threads = 1L,
  n_parameters = NULL,
  stochastic_schedule = NULL,
  ode_control = NULL
)
```

Arguments:

`data` The data set to be used for the particle filter, created by `particle_filter_data()`. This is essentially a `data.frame()` with at least columns `time_start` and `time_end`, along with any additional data used in the `compare` function, and additional information about how your steps relate to time.

`model` A stochastic model to use. Must be a `dust_generator` object.

`compare` A comparison function. Must take arguments `state`, `observed` and `pars` as arguments (though the arguments may have different names). `state` is the simulated model state (a matrix with as many rows as there are state variables and as many columns as there are particles, `data` is a `list` of observed data corresponding to the current time's row in the `data` object provided here in the constructor. `pars` is any additional parameters passed through to the comparison function (via the `pars` argument to `$run`).

`index` An index function. This is used to compute the "interesting" indexes of your model. It must be a function of one argument, which will be the result of calling the `$info()` method on your model. It should return a list with elements `run` (indices to return at the end of each run, passed through to your compare function) and `state` (indices to return if saving state). These indices can overlap but do not have to. This argument is optional but using it will likely speed up your simulation if you have more than a few states as it will reduce the amount of memory copied back and forth.

`initial` A function to generate initial conditions. If given, then this function must accept 3 arguments: `info` (the result of calling `$info()` as for `index`), `n_particles` (the number of particles that the particle filter is using) and `pars` (parameters passed in in the `$run` method via the `pars` argument). It must return a list, which can have the elements `state` (initial model state, passed to the particle filter - either a vector or a matrix, and overriding the initial conditions provided by your model) and `time` (the initial time, overriding the first time step of your data - this must occur within your first epoch in your `data` provided to the constructor, i.e., not less than the first element of `time_start` and not more than `time_end`). Your function can also return a vector or matrix of `state` and not alter the starting time, which is equivalent to returning `list(state = state, time = NULL)`. (TODO: this no longer is allowed, and the docs might be out of date?)

`constant_log_likelihood` An optional function, taking the model parameters, that computes the constant part of the log-likelihood value (if any). You can use this where your likelihood depends both on the time series (via `data`) but also on some non-temporal data. You should

bind any non-parameter dependencies into this closure. This is applied at the beginning of the filter run, so represents the initial condition of the marginal log likelihood value propagated by the process.

`n_threads` Number of threads to use when running the simulation. Defaults to 1, and should not be set higher than the number of cores available to the machine. This currently has no effect as the simulation will be run in serial on a single particle for now.

`n_parameters` Number of parameter sets required. This, along with `data`, controls the interpretation of how the deterministic particle, and importantly will add an additional dimension to most outputs (scalars become vectors, vectors become matrices etc).

`stochastic_schedule` Vector of times to perform stochastic updates, for continuous time models. Note that despite the name, these will be applied deterministically (i.e., replacing the stochastic draw with its expectation).

`ode_control` Tuning control for the ODE stepper, for continuous time (ODE) models

Method `run()`**:** Run the deterministic particle filter

Usage:

```
particle_deterministic$run(
  pars = list(),
  save_history = FALSE,
  save_restart = NULL,
  min_log_likelihood = -Inf
)
```

Arguments:

`pars` A list representing parameters. This will be passed as the `pars` argument to your model, to your `compare` function, and (if using) to your `initial` function. It must be an R list (not vector or `NULL`) because that is what a dust model currently requires on initialisation or `$reset` - we may relax this later. You may want to put your observation and initial parameters under their own keys (e.g., `pars$initial$whatever`), but this is up to you. Extra keys are silently ignored by dust models.

`save_history` Logical, indicating if the history of all particles should be saved. If saving history, then it can be queried later with the `$history` method on the object.

`save_restart` An integer vector of time points to save restart infomation for. Not currently supported.

`min_log_likelihood` Not currently supported, exists to match the inteface with particle_filter. Providing a value larger than -Inf will cause an error.

Returns: A single numeric value representing the log-likelihood (`-Inf` if the model is impossible)

Method `run_begin()`**:** Begin a deterministic run. This is part of the "advanced" interface; typically you will want to use `$run()` which provides a user-facing wrapper around this function. Once created with `$run_begin()`, you should take as many steps as needed with `$step()`.

Usage:

```
particle_deterministic$run_begin(
  pars,
  save_history = FALSE,
  save_restart = NULL,
```

```
  min_log_likelihood = -Inf
)
```

Arguments:

`pars` A list representing parameters. See `$run_many()` for details (and *not* `$run()`)

`save_history` Logical, indicating if the history of all particles should be saved. See `$run()` for details.

`save_restart` Times to save restart state at. See `$run()` for details.

`min_log_likelihood` Not currently supported, exists to match the inteface with particle_filter. Providing a value larger than -Inf will cause an error.

Returns: An object of class `particle_deterministic_state`, with methods `step` and `end`. This interface is still subject to change.

Method `state()`**:** Extract the current model state, optionally filtering. If the model has not yet been run, then this method will throw an error. Returns a matrix with the number of rows being the number of model states, and the number of columns being the number of particles.

Usage:

```
particle_deterministic$state(index_state = NULL)
```

Arguments:

`index_state` Optional vector of states to extract

Method `history()`**:** Extract the particle trajectories. Requires that the model was run with `save_history = TRUE`, which does incur a performance cost. This method will throw an error if the model has not run, or was run without `save_history = TRUE`. Returns a 3d array with dimensions corresponding to (1) model state, filtered by `index$run` if provided, (2) particle (following `index_particle` if provided), (3) time point.

Usage:

```
particle_deterministic$history(index_particle = NULL)
```

Arguments:

`index_particle` Optional vector of particle indices to return. If `NULL` we return all particles' histories.

Method `restart_state()`**:** Return the full particle filter state at points back in time that were saved with the `save_restart` argument to `$run()`. If available, this will return a 3d array, with dimensions representing (1) particle state, (2) particle index, (3) time point. If multiple parameters are used then returns a 4d array, with dimensions representing (1) particle state, (2) particle index, (3) parameter, (4) time point. This could be quite large, especially if you are using the `index` argument to create the particle filter and return a subset of all state generally. In the stochastic version, this is different the saved trajectories returned by `$history()` because earlier saved state is not filtered by later filtering, but in the deterministic model we run with a single particle so it *is* the same.

Usage:

```
particle_deterministic$restart_state(
  index_particle = NULL,
  save_restart = NULL,
  restart_match = FALSE
)
```

Arguments:

`index_particle` Optional vector of particle indices to return. If `NULL` we return all particles' states. Practically because the only valid value of index_particle is "1", this has no effect and it is included primarily for compatibility with the stochastic interface.

Method `inputs()`**:** Return a list of inputs used to configure the deterministic particle filter. These correspond directly to the argument names for the constructor and are the same as the input arguments.

Usage:

```
particle_deterministic$inputs()
```

Method `set_n_threads()`**:** Set the number of threads used by the particle filter (and dust model) after creation. This can be used to allocate additional (or subtract excess) computing power from the deterministic filter Returns (invisibly) the previous value.

Usage:

```
particle_deterministic$set_n_threads(n_threads)
```

Arguments:

`n_threads` The new number of threads to use. You may want to wrap this argument in `dust::dust_openmp_threads()` in order to verify that you can actually use the number of threads requested (based on environment variables and OpenMP support).

`particle_deterministic_state` *Deterministic particle state*

Description

Deterministic particle internal state. This object is not ordinarily constructed directly by users, but via the `$run_begin` method to particle_deterministic. It provides an advanced interface to the deterministic particle that allows partially running over part of the time trajectory.

This state object has a number of public fields that you can read but must not write (they are not read-only so you *could* write them, but don't).

Public fields

`model` The dust model being simulated

`history` The particle history, if created with `save_history = TRUE`.

`restart_state` Full model state at a series of points in time, if the model was created with non-`NULL` `save_restart`. This is a 3d array as described in particle_filter

`log_likelihood` The log-likelihood so far. This starts at 0 when initialised and accumulates value for each step taken.

`current_time_index` The index of the last completed step.

Methods

Public methods:

- particle_deterministic_state$new()
- particle_deterministic_state$run()
- particle_deterministic_state$step()
- particle_deterministic_state$fork_multistage()

Method `new()`**:** Initialise the deterministic particle state. Ordinarily this should not be called by users, and so arguments are barely documented.

Usage:

```
particle_deterministic_state$new(
  pars,
  generator,
  model,
  data,
  data_split,
  times,
  has_multiple_parameters,
  n_threads,
  initial,
  index,
  compare,
  constant_log_likelihood,
  save_history,
  save_restart,
  stochastic_schedule,
  ode_control
)
```

Arguments:

`pars` Parameters for a single phase

`generator` A dust generator object

`model` If the generator has previously been initialised

`data` A particle_filter_data data object

`data_split` The same data as `data` but split by step

`times` A matrix of time step beginning and ends

`has_multiple_parameters` Compute multiple likelihoods at once?

`n_threads` The number of threads to use

`initial` Initial condition function (or `NULL`)

`index` Index function (or `NULL`)

`compare` Compare function

`constant_log_likelihood` Constant log likelihood function

`save_history` Logical, indicating if we should save history

`save_restart` Vector of time steps to save restart at

`stochastic_schedule` Vector of times to perform stochastic updates

`ode_control` Tuning control for stepper

Method `run()`**:** Run the deterministic particle to the end of the data. This is a convenience function around `$step()` which provides the correct value of `time_index`

Usage:

```
particle_deterministic_state$run()
```

Method `step()`**:** Take a step with the deterministic particle. This moves the system forward one step within the *data* (which may correspond to more than one step with your model) and returns the likelihood so far.

Usage:

```
particle_deterministic_state$step(time_index)
```

Arguments:

`time_index` The step *index* to move to. This is not the same as the model step, nor time, so be careful (it's the index within the data provided to the filter). It is an error to provide a value here that is lower than the current step index, or past the end of the data.

Method `fork_multistage()`**:** Create a new `deterministic_particle_state` object based on this one (same model, position in time within the data) but with new parameters, to support the "multistage particle filter".

Usage:

```
particle_deterministic_state$fork_multistage(model, pars, transform_state)
```

Arguments:

`model` A model object

`pars` New model parameters

`transform_state` A function to transform the model state from the old to the new parameter set. See `multistage_epoch()` for details.

`particle_filter` *Particle filter*

Description

Create a `particle_filter` object for running and interacting with a particle filter. A higher-level interface will be implemented later.

Public fields

`model` The dust model generator being simulated (cannot be re-bound)

`n_particles` Number of particles used (read only)

`has_multiple_parameters` Logical, indicating if the particle filter requires multiple parameter sets in a list as inputs, and if it it will produce a vector of likelihoods the same length (read only). The parameter sets may or may not use the same data (see `has_multiple_data`).

has_multiple_data Logical, indicating if the particle filter simultaneously calculates the likelihood for multiple parameter sets (read only). If TRUE, has_multiple_parameters will always be TRUE.

n_parameters The number of parameter sets used by this particle filter (read only). The returned vector of likelihood will be this length, and if has_multiple_parameters is FALSE this will be 1.

n_data The number of data sets used by this particle filter (read only). This will either be 1 or the same value as n_parameters.

Methods

Public methods:

- particle_filter$new()
- particle_filter$run()
- particle_filter$run_begin()
- particle_filter$state()
- particle_filter$history()
- particle_filter$ode_statistics()
- particle_filter$restart_state()
- particle_filter$inputs()
- particle_filter$set_n_threads()

Method new(): Create the particle filter

Usage:

```
particle_filter$new(
  data,
  model,
  n_particles,
  compare,
  index = NULL,
  initial = NULL,
  constant_log_likelihood = NULL,
  n_threads = 1L,
  seed = NULL,
  n_parameters = NULL,
  gpu_config = NULL,
  stochastic_schedule = NULL,
  ode_control = NULL
)
```

Arguments:

data The data set to be used for the particle filter, created by particle_filter_data(). This is essentially a data.frame() with at least columns time_start and time_end, along with any additional data used in the compare function, and additional information about how your dust time steps relate to a more interpretable measure of model time.

model A stochastic model to use. Must be a dust_generator object.

`n_particles` The number of particles to simulate

`compare` A comparison function. Must take arguments `state`, `observed` and `pars` as arguments (though the arguments may have different names). `state` is the simulated model state (a matrix with as many rows as there are state variables and as many columns as there are particles, `data` is a `list` of observed data corresponding to the current time's row in the `data` object provided here in the constructor. `pars` is any additional parameters passed through to the comparison function (via the `pars` argument to `$run`). Alternatively, `compare` can be `NULL` if your model provides a built-in compile compare function (if `model$public_methods$has_compare()` is `TRUE`), which may be faster.

`index` An index function. This is used to compute the "interesting" indexes of your model. It must be a function of one argument, which will be the result of calling the `$info()` method on your model. It should return a list with elements `run` (indices to return at the end of each run, passed through to your compare function) and `state` (indices to return if saving state). These indices can overlap but do not have to. This argument is optional but using it will likely speed up your simulation if you have more than a few states as it will reduce the amount of memory copied back and forth.

`initial` A function to generate initial conditions. If given, then this function must accept 3 arguments: `info` (the result of calling `$info()` as for `index`), `n_particles` (the number of particles that the particle filter is using) and `pars` (parameters passed in in the `$run` method via the `pars` argument). It must return a list, which can have the elements `state` (initial model state, passed to the particle filter - either a vector or a matrix, and overriding the initial conditions provided by your model) and `time` (the initial time step, overriding the first time step of your data - this must occur within your first epoch in your `data` provided to the constructor, i.e., not less than the first element of `time_start` and not more than `time_end`). Your function can also return a vector or matrix of `state` and not alter the starting time step, which is equivalent to returning `list(state = state, time = NULL)`.

`constant_log_likelihood` An optional function, taking the model parameters, that computes the constant part of the log-likelihood value (if any). You can use this where your likelihood depends both on the time series (via `data`) but also on some non-temporal data. You should bind any non-parameter dependencies into this closure. This is applied at the beginning of the filter run, so represents the initial condition of the marginal log likelihood value propagated by the filter.

`n_threads` Number of threads to use when running the simulation. Defaults to 1, and should not be set higher than the number of cores available to the machine.

`seed` Seed for the random number generator on initial creation. Can be `NULL` (to initialise using R's random number generator), a positive integer, or a raw vector - see `dust::dust` and `dust::dust_rng` for more details. Note that the random number stream is unrelated from R's random number generator, except for initialisation with `seed = NULL`.

`n_parameters` Number of parameter sets required. This, along with `data`, controls the interpretation of how the particle filter, and importantly will add an additional dimension to most outputs (scalars become vectors, vectors become matrices etc).

`gpu_config` GPU configuration, typically an integer indicating the device to use, where the model has GPU support. An error is thrown if the device id given is larger than those reported to be available (note that CUDA numbers devices from 0, so that '0' is the first device, so on). See the method `$gpu_info()` for available device ids; this can be called before object creation as `model$public_methods$gpu_info()`. For additional control, provide a list with elements `device_id` and `run_block_size`. Further options (and validation) of this list will be added in a future version!

`stochastic_schedule` Vector of times to perform stochastic updates, for continuous time models.

`ode_control` Tuning control for the ODE stepper, for continuous time (ODE) models

Method `run()`**:** Run the particle filter

Usage:

```
particle_filter$run(
  pars = list(),
  save_history = FALSE,
  save_restart = NULL,
  min_log_likelihood = NULL
)
```

Arguments:

`pars` A list representing parameters. This will be passed as the `pars` argument to your model, to your `compare` function, and (if using) to your `initial` function. It must be an R list (not vector or `NULL`) because that is what a dust model currently requires on initialisation or `$reset` - we may relax this later. You may want to put your observation and initial parameters under their own keys (e.g., `pars$initial$whatever`), but this is up to you. Extra keys are silently ignored by dust models.

`save_history` Logical, indicating if the history of all particles should be saved. If saving history, then it can be queried later with the `$history` method on the object.

`save_restart` An integer vector of time points to save restart infomation for. These are in terms of your underlying time variable (the `time` column in `particle_filter_data()`) not in terms of time steps. The state will be saved after the particle filtering operation (i.e., at the end of the step).

`min_log_likelihood` Optionally, a numeric value representing the smallest likelihood we are interested in. If given and the particle filter drops below this number, then we terminate early and return `-Inf`. In this case, history and final state cannot be returned from the filter. This is primarily intended for use with pmcmc where we can avoid computing likelihoods that will certainly be rejected. Only suitable for use where log-likelihood increments (with the `compare` function) are always negative. This is the case if you use a normalised discrete distribution, but not necessarily otherwise. If using a multi-parameter filter this can be a single number (in which case the exit is when the sum of log-likelihoods drops below this threshold) or a vector of numbers the same length as `pars` (in which case exit occurs when all numbers drop below this threshold).

Returns: A single numeric value representing the log-likelihood (`-Inf` if the model is impossible)

Method `run_begin()`**:** Begin a particle filter run. This is part of the "advanced" interface for the particle filter; typically you will want to use `$run()` which provides a user-facing wrapper around this function. Once created with `$run_begin()`, you should take as many steps as needed with `$step()`.

Usage:

```
particle_filter$run_begin(
  pars = list(),
  save_history = FALSE,
```

```
  save_restart = NULL,
  min_log_likelihood = NULL
)
```

Arguments:

`pars` A list representing parameters. See `$run()` for details.

`save_history` Logical, indicating if the history of all particles should be saved. See `$run()` for details.

`save_restart` Times to save restart state at. See `$run()` for details.

`min_log_likelihood` Optionally, a numeric value representing the smallest likelihood we are interested in. See `$run()` for details.

Returns: An object of class `particle_filter_state`, with methods `step` and `end`. This interface is still subject to change.

Method `state()`**:** Extract the current model state, optionally filtering. If the model has not yet been run, then this method will throw an error. Returns a matrix with the number of rows being the number of model states, and the number of columns being the number of particles.

Usage:

```
particle_filter$state(index_state = NULL)
```

Arguments:

`index_state` Optional vector of states to extract

Method `history()`**:** Extract the particle trajectories. Requires that the model was run with `save_history = TRUE`, which does incur a performance cost. This method will throw an error if the model has not run, or was run without `save_history = TRUE`. Returns a 3d array with dimensions corresponding to (1) model state, filtered by `index$run` if provided, (2) particle (following `index_particle` if provided), (3) time point. If using a multi-parameter filter then returns a 4d array with dimensions corresponding to (1) model state, (2) particle, (3) parameter, (4) time point.

Usage:

```
particle_filter$history(index_particle = NULL)
```

Arguments:

`index_particle` Optional vector of particle indices to return. If using a multi-parameter filter then a vector will be replicated to a matrix with number of columns equal to number of parameters, otherwise a matrix can be supplied. If `NULL` we return all particles' histories.

Method `ode_statistics()`**:** Fetch statistics about steps taken during the integration, by calling through to the `$statistics()` method of the underlying model. This is only available for continuous time (ODE) models, and will error if used with discrete time models.

Usage:

```
particle_filter$ode_statistics()
```

Method `restart_state()`**:** Return the full particle filter state at points back in time that were saved with the `save_restart` argument to `$run()`. If available, this will return a 3d array, with dimensions representing (1) particle state, (2) particle index, (3) time point. If multiple parameters are used then returns a 4d array, with dimensions representing (1) particle state, (2) particle index, (3) parameter set, (4) time point. This could be quite large, especially if you are using the `index`

argument to create the particle filter and return a subset of all state generally. It is also different to the saved trajectories returned by `$history()` because earlier saved state is not filtered by later filtering (in the history we return the tree of history representing the histories of the *final* particles, here we are returning all particles at the requested point, regardless if they appear in the set of particles that make it to the end of the simulation).

Usage:

```
particle_filter$restart_state(
  index_particle = NULL,
  save_restart = NULL,
  restart_match = FALSE
)
```

Arguments:

`index_particle` Optional vector of particle indices to return. If `NULL` we return all particles' states.

Method `inputs()`**:** Return a list of inputs used to configure the particle filter. These correspond directly to the argument names for the particle filter constructor and are the same as the input argument with the exception of `seed`, which is the state of the rng if it has been used (this can be used as a seed to restart the model).

Usage:

```
particle_filter$inputs()
```

Method `set_n_threads()`**:** Set the number of threads used by the particle filter (and dust model) after creation. This can be used to allocate additional (or subtract excess) computing power from a particle filter. Returns (invisibly) the previous value.

Usage:

```
particle_filter$set_n_threads(n_threads)
```

Arguments:

`n_threads` The new number of threads to use. You may want to wrap this argument in `dust::dust_openmp_threads()` in order to verify that you can actually use the number of threads requested (based on environment variables and OpenMP support).

Examples

```
# A basic SIR model included in the dust package
gen <- dust::dust_example("sir")

# Some data that we will fit to, using 1 particle:
sir <- gen$new(pars = list(), time = 0, n_particles = 1)
dt <- 1 / 4
day <- seq(1, 100)
incidence <- rep(NA, length(day))
true_history <- array(NA_real_, c(5, 1, 101))
true_history[, 1, 1] <- sir$state()
for (i in day) {
  state_start <- sir$state()
  sir$run(i / dt)
  state_end <- sir$state()
```

```
  true_history[, 1, i + 1] <- state_end
  # Reduction in S
  incidence[i] <- state_start[1, 1] - state_end[1, 1]
}

# Convert this into our required format:
data_raw <- data.frame(day = day, incidence = incidence)
data <- particle_filter_data(data_raw, "day", 4, 0)

# A comparison function
compare <- function(state, observed, pars = NULL) {
  if (is.null(pars$exp_noise)) {
    exp_noise <- 1e6
  } else {
    exp_noise <- pars$exp_noise
  }
  incidence_modelled <- state[1,]
  incidence_observed <- observed$incidence
  lambda <- incidence_modelled +
    rexp(length(incidence_modelled), exp_noise)
  dpois(incidence_observed, lambda, log = TRUE)
}

# Construct the particle_filter object with 100 particles
p <- particle_filter$new(data, gen, 100, compare)
p$run(save_history = TRUE)

# Our simulated trajectories, with the "real" data superimposed
history <- p$history()
matplot(data_raw$day, t(history[1, , -1]), type = "l",
        xlab = "Time", ylab = "State",
        col = "#ff000022", lty = 1, ylim = range(history))
matlines(data_raw$day, t(history[2, , -1]), col = "#ffff0022", lty = 1)
matlines(data_raw$day, t(history[3, , -1]), col = "#0000ff22", lty = 1)
matpoints(data_raw$day, t(true_history[1:3, , -1]), pch = 19,
          col = c("red", "yellow", "blue"))
```

`particle_filter_data` *Prepare data for use with particle filter*

Description

Prepare data for use with the `particle_filter`. This function is required to use the particle filter as helps arrange data and be explicit about the off-by-one errors that can occur. It takes as input your data to compare against a model, including some measure of "time". We need to convert this time into model time steps (see Details).

Usage

```
particle_filter_data(data, time, rate, initial_time = NULL, population = NULL)
```

Arguments

data	A data.frame() of data
time	The name of a column within data that represents your measure of time. This column must be integer-like. To avoid confusion, this cannot be called step, time, or model_time.
rate	The number of model "time steps" that occur between each time point (in model time time). This must also be integer-like for discrete time models and must be NULL for continuous time models.
initial_time	An initial time to start the model from. This should always be provided, and must be provided for continuous time models. For discrete time models, this is expressed in model time. It must be a non-negative integer and must be at most equal to the first value of the time column, minus 1 (i.e., data[[time]] - 1). For historical reasons if not given we take the first value of the time column minus one, but with a warning - this behaviour will be removed in a future version of mcstate.
population	Optionally, the name of a column within data that represents different populations. Must be a factor.

Details

We require that the time variable increments in unit steps; this may be relaxed in future to even steps, or possibly irregular steps, but for now this assumption is required. We assume that the data in the first column is recorded at the end of a period of 1 time unit. So if you have in the first column `t = 10, data = 100` we assume that the model steps from `t = 9` to to `t = 10` and at that period the data has value 100.

For continuous time models, time is simple to think about; time is continuous (and real-valued) and really any time is acceptable. For discrete time models there are two correlated measures of time we need to consider - (1) the dust "time step", a non-negative integer value that increases in unit steps, and (2) the "model time" which is related to the dust time step based on the rate parameter here as <model time> = <dust time> * <rate>. For a concrete example, consider a model where we want to think in terms of days, but which we take 10 steps per day. Time step 0 and model time 0 are the same, but day 1 occurs at step 10, day 15 at step 150 and so on.

Value

If population is NULL, a data.frame with new columns time_start and time_end (required by particle_filter), along side all previous data except for the time variable, which is replaced by new <time>_start and <time>_end columns. If population is not NULL then a named list of data.frames as described above where each element represents populations in the order specified in the data.

Examples

```
d <- data.frame(day = 5:20, y = runif(16))
mcstate::particle_filter_data(d, "day", rate = 4, initial_time = 4)

# If providing an initial day, then the first epoch of simulation
```

```
# will be longer (see the first row)
mcstate::particle_filter_data(d, "day", rate = 4, initial_time = 0)

# If including populations:
d <- data.frame(day = 5:20, y = runif(16),
                population = factor(rep(letters[1:2], each = 16)))
mcstate::particle_filter_data(d, "day", 4, 0, "population")
```

`particle_filter_initial` *Create restart initial state*

Description

Create a suitable initial condition function from a set of restart state. This takes care of a few bookkeping and serialisation details and returns a function appropriate to pass to particle_filter as `initial`.

Usage

```
particle_filter_initial(state)
```

Arguments

`state`	A matrix of state (rows are different states, columns are different realisations). This is the form of a slice pulled from a restart.

Value

A function with arguments `info`, `n_particles` and `pars` that will sample, with replacement, a matrix of state suitable as a starting point for a particle filter. The `info` and `pars` arguments are ignored.

`particle_filter_state` *Particle filter state*

Description

Particle filter internal state. This object is not ordinarily constructed directly by users, but via the `$run_begin` method to particle_filter. It provides an advanced interface to the particle filter that allows partially running the particle filter over part of the time trajectory.

This state object has a number of public fields that you can read but must not write (they are not read-only so you *could* write them, but don't).

Public fields

`model` The dust model being simulated

`history` The particle history, if created with `save_history = TRUE`. This is an internal format subject to

`restart_state` Full model state at a series of points in time, if the model was created with non-`NULL` `save_restart`. This is a 3d (or greater) array as described in particle_filter

`log_likelihood` The log-likelihood so far. This starts at 0 when initialised and accumulates value for each step taken.

`log_likelihood_step` The log-likelihood attributable to the last step (i.e., the contribution to `log_likelihood` made on the last call to `$step()`.

`current_time_index` The index of the last completed step.

Methods

Public methods:

- particle_filter_state$new()
- particle_filter_state$run()
- particle_filter_state$step()
- particle_filter_state$fork_multistage()
- particle_filter_state$fork_smc2()

Method `new()`**:** Initialise the particle filter state. Ordinarily this should not be called by users, and so arguments are barely documented.

Usage:

```
particle_filter_state$new(
  pars,
  generator,
  model,
  data,
  data_split,
  times,
  n_particles,
  has_multiple_parameters,
  n_threads,
  initial,
  index,
  compare,
  constant_log_likelihood,
  gpu_config,
  seed,
  min_log_likelihood,
  save_history,
  save_restart,
  stochastic_schedule,
  ode_control
)
```

Arguments:

`pars` Parameters for a single phase

`generator` A dust generator object

`model` If the generator has previously been initialised

`data` A particle_filter_data data object

`data_split` The same data as `data` but split by step

`times` A matrix of time step beginning and ends

`n_particles` Number of particles to use

`has_multiple_parameters` Compute multiple likelihoods at once?

`n_threads` The number of threads to use

`initial` Initial condition function (or `NULL`)

`index` Index function (or `NULL`)

`compare` Compare function

`constant_log_likelihood` Constant log likelihood function

`gpu_config` GPU configuration, passed to `generator`

`seed` Initial RNG seed

`min_log_likelihood` Early termination control

`save_history` Logical, indicating if we should save history

`save_restart` Vector of time steps to save restart at

`stochastic_schedule` Vector of times to perform stochastic updates

`ode_control` Tuning control for stepper

Method `run()`**:** Run the particle filter to the end of the data. This is a convenience function around `$step()` which provides the correct value of `time_index`

Usage:

```
particle_filter_state$run()
```

Method `step()`**:** Take a step with the particle filter. This moves the particle filter forward one step within the *data* (which may correspond to more than one step with your model) and returns the likelihood so far.

Usage:

```
particle_filter_state$step(time_index, partial = FALSE)
```

Arguments:

`time_index` The step *index* to move to. This is not the same as the model step, nor time, so be careful (it's the index within the data provided to the filter). It is an error to provide a value here that is lower than the current step index, or past the end of the data.

`partial` Logical, indicating if we should return the partial likelihood, due to this step, rather than the full likelihood so far.

Method `fork_multistage()`**:** Create a new `particle_filter_state` object based on this one (same model, position in time within the data) but with new parameters, to support the "multistage particle filter". Unlike `fork_smc2`, here the parameters may imply a different model shape and arbitrary transformations of the state are allowed. The model is not rerun to the current point, just transformed at that point.

Usage:

```
particle_filter_state$fork_multistage(model, pars, transform_state)
```

Arguments:

`model` A model object (or NULL)

`pars` New model parameters

`transform_state` A function to transform the model state from the old to the new parameter set. See `multistage_epoch()` for details.

Method `fork_smc2()`**:** Create a new `particle_filter_state` object based on this one (same model, position in time within the data) but with new parameters, run up to the date, to support the `smc2()` algorithm. To do this, we create a new `particle_filter_state` with new parameters at the beginning of the simulation (corresponding to the start of your data or the `initial` argument to particle_filter) with your new `pars`, and then run the filter foward in time until it reaches the same step as the parent model.

Usage:

```
particle_filter_state$fork_smc2(pars)
```

Arguments:

`pars` New model parameters

`pmcmc` *Run a pmcmc sampler*

Description

Run a pmcmc sampler

Usage

```
pmcmc(pars, filter, initial = NULL, control = NULL)
```

Arguments

`pars`	A `pmcmc_parameters` object containing information about parameters (ranges, priors, proposal kernel, translation functions for use with the particle filter).
`filter`	A `particle_filter` object
`initial`	Optional initial starting point. If given, it must be compatible with the parameters given in `pars`, and must be valid against your prior. You can use this to override the initial conditions saved in your `pars` object. You can provide either a vector of initial conditions, or a matrix with `n_chains` columns to use a different starting point for each chain.
`control`	A pmcmc_control object which will control how the MCMC runs, including the number of steps etc.

Details

This is a basic Metropolis-Hastings MCMC sampler. The `filter` is run with a set of parameters to evaluate the likelihood. A new set of parameters is proposed, and these likelihoods are compared, jumping with probability equal to their ratio. This is repeated for `n_steps` proposals.

While this function is called `pmcmc` and requires a particle filter object, there's nothing special about it for particle filtering. However, we may need to add things in the future that make assumptions about the particle filter, so we have named it with a "p".

Value

A `mcstate_pmcmc` object containing `pars` (sampled parameters) and `probabilities` (log prior, log likelihood and log posterior values for these probabilities). Two additional fields may be present: `state` (if `return_state` was `TRUE`), containing the final state of a randomly selected particle at the end of the simulation, for each step (will be a matrix with as many rows as your state has variables, and as `n_steps + 1` columns corresponding to each step). `trajectories` will include a 3d array of particle trajectories through the simulation (if `return_trajectories` was `TRUE`).

`pmcmc_chains_prepare` *pMCMC with manual chain scheduling*

Description

Run a pMCMC, with sensible random number behaviour, but schedule execution of the chains yourself. Use this if you want to distribute chains over (say) the nodes of an HPC system.

Usage

```
pmcmc_chains_prepare(path, pars, filter, control, initial = NULL)

pmcmc_chains_run(chain_id, path, n_threads = NULL)

pmcmc_chains_collect(path)

pmcmc_chains_cleanup(path)
```

Arguments

`path`	The path to use to exchange inputs and results. You can use a temporary directory or a different path (relative or absolute). Several rds files will be created. It is strongly recommended not to use `.`
`pars`	A `pmcmc_parameters` object containing information about parameters (ranges, priors, proposal kernel, translation functions for use with the particle filter).
`filter`	A `particle_filter` object
`control`	A pmcmc_control object which will control how the MCMC runs, including the number of steps etc.

initial	Optional initial starting point. If given, it must be compatible with the parameters given in pars, and must be valid against your prior. You can use this to override the initial conditions saved in your pars object. You can provide either a vector of initial conditions, or a matrix with n_chains columns to use a different starting point for each chain.
chain_id	The integer identifier of the chain to run
n_threads	Optional thread count, overriding the number set in the control. This will be useful where preparing the threads on a machine with one level of resource and running it on another.

Details

Basic usage will look like

```
path <- mcstate::pmcmc_chains_prepare(tempfile(), pars, filter, control)
for (i in seq_len(control$n_chains)) {
  mcstate::pmcmc_chains_run(i, path)
}
samples <- mcstate::pmcmc_chains_collect(path)
mcstate::pmcmc_chains_cleanup(path)
```

You can safely parallelise (or not) however you like at the point where the loop is (even across other machines) and get the same outputs regardless.

---

pmcmc_combine *Combine pmcmc samples*

Description

Combine multiple pmcmc() samples into one object

Usage

```
pmcmc_combine(..., samples = list(...))
```

Arguments

...	Arguments representing pmcmc() sample, i.e., mcstate_pmcmc objects. Alternatively, pass a list as the argument samples. Names are ignored.
samples	A list of mcstate_pmcmc objects. This is often more convenient for programming against than ...

`pmcmc_control` *Control for the pmcmc*

Description

Control for the pmcmc. This function constructs a list of options and does some basic validation to ensure that the options will work well together. Do not manually change the values in this object. Do not refer to any argument except `n_steps` by position as the order of the arguments may change in future.

Usage

```
pmcmc_control(
  n_steps,
  n_chains = 1L,
  n_threads_total = NULL,
  n_workers = 1L,
  rerun_every = Inf,
  rerun_random = FALSE,
  use_parallel_seed = FALSE,
  save_state = TRUE,
  save_restart = NULL,
  save_trajectories = FALSE,
  progress = FALSE,
  nested_step_ratio = 1,
  nested_update_both = FALSE,
  filter_early_exit = FALSE,
  restart_match = FALSE,
  n_burnin = NULL,
  n_steps_retain = NULL,
  adaptive_proposal = NULL,
  path = NULL
)
```

Arguments

`n_steps`	Number of MCMC steps to run. This is the only required argument.
`n_chains`	Optional integer, indicating the number of chains to run. If more than one then we run a series of chains and merge them with `pmcmc_combine()`. Chains are run in series, with the same filter if `n_workers` is 1, or run in parallel otherwise.
`n_threads_total`	The total number of threads (i.e., cores) the total number of threads/cores to use. If `n_workers` is greater than 1 then these threads will be divided evenly across your workers at first and so `n_threads_total` must be an even multiple of `n_workers`. If `n_chains` is not a clean multiple of `n_workers` we will try and allocate the leftover threads evenly across the last wave of chains. This

value must be provided if `n_workers` is given, but is optional otherwise - if given it overrides the value in the particle filter.

`n_workers` Number of "worker" processes to use to run chains in parallel. This must be at most `n_chains` and is recommended to be a divisor of `n_chains`. If `n_workers` is 1, then chains are run in series (i.e., one chain after the other). See the parallel vignette (`vignette("parallelisation", package = "mcstate")`) for more details about this approach.

`rerun_every` Optional integer giving the frequency at which we should rerun the particle filter on the current "accepted" state. The default for this (`Inf`) will never rerun this point, but if you set to 100, then every 100 steps we run the particle filter on both the proposed *and* previously accepted point before doing the comparison. This may help "unstick" chains, at the cost of some bias in the results.

`rerun_random` Logical, controlling the behaviour of rerunning (when `rerun_every` is finite). The default value of `FALSE` will rerun the filter deterministically at a fixed number of iterations (given by `rerun_every`). If `TRUE`, then we stochastically rerun each step with probability of `1 / rerun_every`. This gives the same expected number of MCMC steps between reruns but a different pattern.

`use_parallel_seed`
Logical, indicating if seeds should be configured in the same way as when running workers in parallel (with `n_workers > 1`). Set this to `TRUE` to ensure reproducibility if you use this option sometimes (but not always). This option only has an effect if `n_workers` is 1.

`save_state` Logical, indicating if the state should be saved at the end of the simulation. If `TRUE`, then a single randomly selected particle's state will be collected at the end of each MCMC step. This is the full state (i.e., unaffected by and `index` used in the particle filter) so that the process may be restarted from this point for projections. If `save_trajectories` is `TRUE` the same particle will be selected for each. The default is `TRUE`, which will cause `n_state * n_steps` of data to be output alongside your results. Set this argument to `FALSE` to save space, or use `pmcmc_thin()` after running the MCMC.

`save_restart` An integer vector of time points to save restart information for; this is in addition to `save_state` (which saves the final model state) and saves the full model state. It will use the same trajectory as `save_state` and `save_trajectories`. Note that if you use this option you will end up with lots of model states and will need to process them in order to actually restart the pmcmc or the particle filter from this state. The integers correspond to the *time* variable in your filter (see particle_filter for more information).

`save_trajectories`
Logical, indicating if the particle trajectories should be saved during the simulation. If `TRUE`, then a single randomly selected particle's trajectory will be collected at the end of each MCMC step. This is the filtered state (i.e., using the `state` component of `index` provided to the particle filter). If `save_state` is `TRUE` the same particle will be selected for each.

`progress` Logical, indicating if a progress bar should be displayed, using `progress::progress_bar`.

`nested_step_ratio`
Either integer or 1/integer, which specifies the ratio of fixed:varied steps in a nested pMCMC. For example `3` would run 3 steps proposing fixed parameters

only and then 1 step proposing varied parameters only; whereas `1/3` would run 3 varied steps for every 1 fixed step. The default value of 1 runs an equal number of iterations updating the fixed and varied parameters. Sensible choices of this parameter may depend on the true ratio of fixed:varied parameters or on desired run-time, for example updating fixed parameters is quicker so more varied steps could be more efficient.

`nested_update_both`
: If `FALSE` (default) then alternates between proposing fixed and varied parameter updates according to the ratio in `nested_step_ratio`. If `TRUE` then proposes fixed and varied parameters simultaneously and collectively accepts/rejects them, `nested_step_ratio` is ignored.

`filter_early_exit`
: Logical, indicating if we should allow the particle filter to exit early for points that will not be accepted. Only use this if your log-likelihood never increases between steps. This will the the case where your likelihood calculation is a sum of discrete normalised probability distributions, but may not be for continuous distributions!

`restart_match`
: Logical, indicating whether the restart state saved from the particle filter should match the trajectory saved, otherwise the restart state will be randomly drawn from the states of the particle filter after filtering to the restart time point.

`n_burnin`
: Optionally, the number of points to discard as burnin. This happens separately to the burnin in pmcmc_thin or pmcmc_sample. See Details.

`n_steps_retain`
: Optionally, the number of samples to retain from the `n_steps - n_burnin` steps. See Details.

`adaptive_proposal`
: Optionally, control over an adaptive proposal (adaptive_proposal_control). Alternatively `FALSE` to disable, `TRUE` to enable defaults. This is only valid for single-population deterministic models.

`path`
: Optional path to save partial pmcmc results in, when using workers. If not given (or `NULL`) then a temporary directory is used.

Details

pMCMC is slow and you will want to parallelise it if you possibly can. There are two ways of doing this which are discussed in some detail in `vignette("parallelisation", package = "mcstate")`.

Value

A `pmcmc_control` object, which should not be modified once created.

Thinning the chain at generation

Generally it may be preferable to thin the chains after generation using pmcmc_thin or pmcmc_sample. However, waiting that long can create memory consumption issues because the size of the trajectories can be very large. To avoid this, you can thin the chains at generation - this will avoid creating large trajectory arrays, but will discard some information irretrivably.

If either of the options n_burnin or n_steps_retain are provided, then we will subsample the chain at generation.

- If n_burnin is provided, then the first n_burnin (of n_steps) samples is discarded. This must be at most n_steps
- If n_steps_retain is provided, then we *evenly* sample out of the remaining samples. The algorithm will try and generate a sensible set here, and will always include the last sample of n_steps but may not always include the first post-burnin sample. An error will be thrown if a suitable sampling is not possible (e.g., if n_steps_retain is larger than n_steps - n_burnin

If either of n_burnin or n_steps_retain is provided, the resulting samples object will include the full set of parameters and probabilities sampled, along with an index showing how they relate to the filtered samples.

Examples

```
mcstate::pmcmc_control(1000)

# Suppose we have a fairly large node with 16 cores and we want to
# run 8 chains. We can use all cores for a single chain and run
# the chains sequentially like this:
mcstate::pmcmc_control(1000, n_chains = 8, n_threads_total = 16)

# However, on some platforms (e.g., Windows) this may only realise
# a 50% total CPU use, in which case you might benefit from
# splitting these chains over different worker processes (2-4
# workers is likely the largest useful number).
mcstate::pmcmc_control(1000, n_chains = 8, n_threads_total = 16,
                       n_workers = 4)
```

---

pmcmc_parameter *Describe single pmcmc parameter*

Description

Describe a single parameter for use within the pmcmc. Note that the name is not set here, but will end up being naturally defined when used with pmcmc_parameters, which collects these together for use with pmcmc().

Usage

```
pmcmc_parameter(
  name,
  initial,
  min = -Inf,
  max = Inf,
  discrete,
  integer = FALSE,
  prior = NULL,
```

```
  mean = NULL
)
```

Arguments

name	Name for the parameter (a string)
initial	Initial value for the parameter
min	Optional minimum value for the parameter (otherwise -Inf). If given, then initial must be at least this value.
max	Optional max value for the parameter (otherwise Inf). If given, then initial must be at most this value.
discrete	Deprecated; use integer instead.
integer	Logical, indicating if this parameter is integer. If TRUE then the parameter will be rounded after a new parameter is proposed.
prior	A prior function (if not given an improper flat prior is used - be careful!). It must be a function that takes a single argument, being the value of this parameter. If given, then prior(initial) must evaluate to a finite value.
mean	Optionally, an estimate of the mean of the parameter. If not given, then we assume that initial is a reasonable estimate. This is used only in adaptive mcmc.

Examples

```
pmcmc_parameter("a", 0.1)
```

---

pmcmc_parameters *pmcmc_parameters*

Description

Construct parameters for use with pmcmc(). This creates a utility object that is used internally to work with parameters. Most users only need to construct this object, but see the examples for how it can be used.

Parameter transformations

Unless you have a very simple model, it is highly unlikely that the parameters that you are interested in performing inference on are the same as the parameters that you might need to initialise your model.

Due to the nature of mcmc and other inference algorithms, the general assumption is that the inference parameters will be a simple vector of real values; here each of the parameters elements corresponds to one of these. The proposal matrix maps one vector to another via a simple multivariate-gaussian kernel.

On the other hand, dust models can take a named list of arbitrary data as their input parameters (see dust::dust_generator). These might include:

- things that are not parameters at all from the perspective of the inference - for example some quantity that you might vary depending on the region/species/etc you're running the model for but that you are not fitting.
- non-scalar quantities that are directly derived from some parameters that you are fitting. As an example of this, in sircovid, a transmission model of COVID, we take a number of "contact rates" which apply at different points in time, and generate from this an interpolated series of contact rates per time step (a very long vector). Other users have needed to generate equilibrium solutions to parts of their model and used these at initialisation.
- arbitrary complex inputs to the model, for example weather data, demographic matrices, population contact rate matrices etc. These are all "parameters" from the perspective of a dust model but not at all from the perspective of the inference process.

To allow for this in a flexible way, mcstate allows a "transform" function, the `transform` argument to the constructor. This function maps a named numeric vector of inference parameters to whatever you need for your dust model. The default value for this function is as.list which just converts the named vector to a named list, which works well in the example cases here.

When providing a transformation function, you may want to provide a "closure" rather than a top-level function. This way you can bind additional data into your function. For example, suppose that you want to use some demographic matrix `m` in your model, and perform inference on parameters `a` and `b` you might write

```
make_transform <- function(m) {
  function(theta) {
    c(list(m = m), as.list(theta))
  }
}
```

and pass this into `mcstate::pmcmc_parameters$new`, providing parameter definitions only for `a` and `b`. See the examples for full working of this.

Methods

Public methods:

- `pmcmc_parameters$new()`
- `pmcmc_parameters$initial()`
- `pmcmc_parameters$mean()`
- `pmcmc_parameters$vcv()`
- `pmcmc_parameters$names()`
- `pmcmc_parameters$summary()`
- `pmcmc_parameters$prior()`
- `pmcmc_parameters$propose()`
- `pmcmc_parameters$model()`
- `pmcmc_parameters$fix()`

Method `new()`**:** Create the pmcmc_parameters object

Usage:

```
pmcmc_parameters$new(parameters, proposal, transform = NULL)
```

Arguments:

`parameters` A `list` of pmcmc_parameter objects, each of which describe a single parameter in your model. If `parameters` is named, then these names must match the `$name` element of each parameter is used (this is verified).

`proposal` A square proposal distribution corresponding to the variance-covariance matrix of a multivariate gaussian distribution used to generate new parameters. It must have the same number of rows and columns as there are elements in `parameters`, and if named the names must correspond exactly to the names in `parameters`. Because it corresponds to a variance-covariance matrix it must be symmetric and positive definite.

`transform` An optional transformation function to apply to your parameter vector immediately before passing it to the model function. If not given, then as.list is used, as dust models require this. However, if t you need to generate derived parameters from those being actively sampled you can do arbitrary transformations here.

Method `initial()`**:** Return the initial parameter values as a named numeric vector

Usage:

```
pmcmc_parameters$initial()
```

Method `mean()`**:** Return the estimate of the mean of the parameters, as set when created (this is not updated by any fitting!)

Usage:

```
pmcmc_parameters$mean()
```

Method `vcv()`**:** Return the variance-covariance matrix used for the proposal.

Usage:

```
pmcmc_parameters$vcv()
```

Method `names()`**:** Return the names of the parameters

Usage:

```
pmcmc_parameters$names()
```

Method `summary()`**:** Return a `data.frame` with information about parameters (name, min, max, and integer).

Usage:

```
pmcmc_parameters$summary()
```

Method `prior()`**:** Compute the prior for a parameter vector

Usage:

```
pmcmc_parameters$prior(theta)
```

Arguments:

`theta` a parameter vector in the same order as your parameters were defined in (see `$names()` for that order.

Method `propose()`**:** Propose a new parameter vector given a current parameter vector. This proposes a new parameter vector given your current vector and the variance-covariance matrix of your proposal kernel, rounds any integer values, and reflects bounded parameters until they lie within `min`:`max`.

Usage:

```
pmcmc_parameters$propose(theta, scale = 1, vcv = NULL)
```

Arguments:

`theta` a parameter vector in the same order as your parameters were defined in (see `$names()` for that order.

`scale` an optional scaling factor to apply to the proposal distribution. This may be useful in sampling starting points. The parameter is equivalent to a multiplicative factor applied to the variance covariance matrix.

`vcv` A variance covariance matrix of the correct size, overriding the proposal matrix built into the parameters object. This will be slightly less efficient but allow a different proposal matrix to be used (e.g., during an adaptive MCMC)

Method `model()`**:** Apply the model transformation function to a parameter vector.

Usage:

```
pmcmc_parameters$model(theta)
```

Arguments:

`theta` a parameter vector in the same order as your parameters were defined in (see `$names()` for that order.

Method `fix()`**:** Set some parameters to fixed values. Use this to reduce the dimensionality of your system.

Usage:

```
pmcmc_parameters$fix(fixed)
```

Arguments:

`fixed` a named vector of parameters to fix

Examples

```
# Construct an object with two parameters:
pars <- mcstate::pmcmc_parameters$new(
  list(mcstate::pmcmc_parameter("a", 0.1, min = 0, max = 1,
                                prior = function(a) log(a)),
       mcstate::pmcmc_parameter("b", 0, prior = dnorm)),
  matrix(c(1, 0.5, 0.5, 2), 2, 2))

# Initial parameters
p <- pars$initial()
p

# Propose a new parameter point
pars$propose(p)

# Information about parameters:
```

```
pars$names()
pars$summary()

# Compute prior
pars$prior(p)

# Transform data for your model
pars$model(p)

# Above we describe a nontrivial transformation function using a closure
make_transform <- function(m) {
  function(theta) {
    c(list(m = m), as.list(theta))
  }
}

# Suppose this is our demographic matrix (note here that the name
# need not match that used in the transform)
demographic_matrix <- diag(4)

# Construct the parameters as above, but this time passing in the
# function that make_transform returns
pars <- mcstate::pmcmc_parameters$new(
  list(mcstate::pmcmc_parameter("a", 0.1, min = 0, max = 1,
                                prior = function(a) log(a)),
       mcstate::pmcmc_parameter("b", 0, prior = dnorm)),
  matrix(c(1, 0.5, 0.5, 2), 2, 2),
  make_transform(demographic_matrix))

# Now, as above we start from a position in terms of a and b only:
pars$initial()

# But when prepared for the model, our matrix will be set up
pars$model(pars$initial())
```

`pmcmc_parameters_nested`

pmcmc_parameters_nested

Description

Construct nested parameters for use with `pmcmc()`. This creates a utility object that is used internally to work with parameters that may be fixed and the same for all given populations, or varied and possibly-different between populations. Most users only need to construct this object, but see the examples for how it can be used.

Methods

Public methods:

- pmcmc_parameters_nested$new()
- pmcmc_parameters_nested$names()
- pmcmc_parameters_nested$populations()
- pmcmc_parameters_nested$validate()
- pmcmc_parameters_nested$summary()
- pmcmc_parameters_nested$initial()
- pmcmc_parameters_nested$mean()
- pmcmc_parameters_nested$vcv()
- pmcmc_parameters_nested$prior()
- pmcmc_parameters_nested$propose()
- pmcmc_parameters_nested$model()
- pmcmc_parameters_nested$fix()

Method `new()`**:** Create the pmcmc_parameters object

Usage:

```
pmcmc_parameters_nested$new(
  parameters,
  proposal_varied = NULL,
  proposal_fixed = NULL,
  populations = NULL,
  transform = NULL
)
```

Arguments:

`parameters` A `list` of pmcmc_parameter or pmcmc_varied_parameter objects, each of which describe a single (possibly-varying) parameter in your model. If `parameters` is named, then these names must match the `$name` element of each parameter that is used (this is verified).

`proposal_varied, proposal_fixed` Square proposal matrices corresponding to the variance-covariance matrix of a multivariate gaussian distribution used to generate new varied and fixed parameters respectively.'. They must have the same number of rows and columns as there are varied and fixed parameters respectively. The names must correspond exactly to the names in `parameters`. Because it corresponds to a variance-covariance matrix it must be symmetric and positive definite.

`populations` Specifies the names of the different populations that the varying parameters change according to. Only required if no pmcmc_varied_parameter objects are included in `parameters`. Otherwise population names are taken from those objects.

`transform` An optional transformation function to apply to your parameter vector immediately before passing it to the model function. If not given, then as.list is used, as dust models require this. However, if you need to generate derived parameters from those being actively sampled you can do arbitrary transformations here.

Method `names()`**:** Return the names of the parameters

Usage:

```
pmcmc_parameters_nested$names(type = "both")
```

Arguments:

type One of "both" (the default, all parameters), "fixed" (parameters that are shared across populations) or "varied" (parameters that vary over populations).

Method `populations()`**:** Return the names of the populations

Usage:

```
pmcmc_parameters_nested$populations()
```

Method `validate()`**:** Validate a parameter matrix. This method checks that your matrix has the expected size (rows according to parameters, columns to populations) and if named that the names are exactly what is expected. It also verifies that the fixed parameters are same across all populations.

Usage:

```
pmcmc_parameters_nested$validate(theta)
```

Arguments:

`theta` a parameter matrix

Method `summary()`**:** Return a `data.frame` with information about parameters (name, min, max, integer, type (fixed or varied) and population)

Usage:

```
pmcmc_parameters_nested$summary()
```

Method `initial()`**:** Return the initial parameter values as a named matrix with rows corresponding to parameters and columns to populations.

Usage:

```
pmcmc_parameters_nested$initial()
```

Method `mean()`**:** Return the estimate of the mean of the parameters, as set when created (this is not updated by any fitting!)

Usage:

```
pmcmc_parameters_nested$mean(type)
```

Method `vcv()`**:** Return the variance-covariance matrix used for the proposal.

Usage:

```
pmcmc_parameters_nested$vcv(type)
```

Method `prior()`**:** Compute the prior(s) for a parameter matrix. Returns a named vector with names corresponding to populations.

Usage:

```
pmcmc_parameters_nested$prior(theta)
```

Arguments:

`theta` a parameter matrix with columns in the same order as `$names()` and rows in the same order as `$populations()`.

Method `propose()`**:** This proposes a new parameter matrix given your current matrix and the variance-covariance matrices of the proposal kernels, rounds any integer values, and reflects bounded parameters until they lie within `min`:`max`. Returns matrix with rows corresponding to parameters and columns to populations (i.e., the same orientation as `theta`).

Usage:

```
pmcmc_parameters_nested$propose(theta, type, scale = 1, vcv = NULL)
```

Arguments:

`theta` a parameter matrix with rows in the same order as `$names()` and columns in the same order as `$populations()`.

`type` specifies which type of parameters should be proposed, either fixed parameters only ("fixed"), varied only ("varied"), or both ("both") types. For 'fixed' and 'varied', parameters of the other type are left unchanged.

`scale` an optional scaling factor to apply to the proposal distribution. This may be useful in sampling starting points. The parameter is equivalent to a multiplicative factor applied to the variance covariance matrix.

Method `model()`**:** Apply the model transformation function to a parameter matrix.

Usage:

```
pmcmc_parameters_nested$model(theta)
```

Arguments:

`theta` a parameter matrix with rows in the same order as `$names()` and columns in the same order as `$populations()`.

Method `fix()`**:** Set some parameters to fixed values. Use this to reduce the dimensionality of your system. Note that this function has an unfortunate name collision - we use "fixed" and "varied" parameters generally to refer to ones that are fixed across populations or which vary among populations. However, in the context of this method "fixed" refers to parameters which will be set to a single value and no longer used in inference.

Usage:

```
pmcmc_parameters_nested$fix(fixed)
```

Arguments:

`fixed` a named vector of parameters to fix

Examples

```
# Construct an object with two varied parameters ('a' and 'b'),
# two fixed parameters ('c' and 'd') and two populations ('p1' and 'p2')
parameters <- list(mcstate::pmcmc_varied_parameter("a", c("p1", "p2"), 2),
                   mcstate::pmcmc_varied_parameter("b", c("p1", "p2"), 2),
                   mcstate::pmcmc_parameter("c", 3),
                   mcstate::pmcmc_parameter("d", 4))
proposal_fixed <- diag(2)
proposal_varied <- diag(2) + 1
pars <- mcstate::pmcmc_parameters_nested$new(parameters, proposal_varied,
                                             proposal_fixed)

# Initial parameters
p <- pars$initial()
p

# Propose a new parameter point
```

```
pars$propose(p, type = "both")
pars$propose(p, type = "fixed")
pars$propose(p, type = "varied")

# Information about parameters:
pars$names()
pars$names("fixed")
pars$names("varied")
pars$summary()

# Compute log prior probability, per population
pars$prior(p)

# Transform data for your model
pars$model(p)
```

`pmcmc_predict` *Run predictions from PMCMC*

Description

Run predictions from the results of `pmcmc()`. This function can also be called by running `predict()` on the object, using R's S3 dispatch.

Usage

```
pmcmc_predict(
  object,
  times,
  prepend_trajectories = FALSE,
  n_threads = NULL,
  seed = NULL
)
```

Arguments

`object`	The results of running `pmcmc()` with `return_state = TRUE` (without this extra information, prediction is not possible)
`times`	A vector of time times to return predictions for. The first value must be the final value run in your simulation. An error will be thrown if you get this value wrong, look in `object$predict$time` (or the error message) for the correct value.
`prepend_trajectories`	Prepend trajectories from the particle filter to the predictions created here.
`n_threads`	The number of threads used in the simulation. If not given, we default to the value used in the particle filter that was used in the pmcmc.

seed — The random number seed (see particle_filter). The default value of NULL will seed the dust random number generator from R's random number generator. However, you can pick up from the same RNG stream used in the simulation if you pass in seed = object$predict$seed. However, do not do this if you are gong to run pmcmc_predict() multiple times the result will be identical. If you do want to call predict with this state multiple times you should create a persistant rng state object (e.g., with dust::dust_rng and perform a "long jump" between each call.

---

pmcmc_thin *Thin a pmcmc chain*

Description

Thin results of running pmcmc(). This function may be useful before using pmcmc_predict(), or before saving pmcmc output to disk. pmcmc_thin takes every thin'th sample, while pmcmc_sample randomly selects a total of n_sample samples.

Usage

```
pmcmc_thin(object, burnin = NULL, thin = NULL)

pmcmc_sample(object, n_sample, burnin = NULL)
```

Arguments

object — Results of running pmcmc()

burnin — Optional integer number of iterations to discard as "burn-in". If given then samples 1:burnin will be excluded from your results. It is an error if this is not a positive integer or is greater than or equal to the number of samples (i.e., there must be at least one sample remaining after discarding burnin).

thin — Optional integer thinning factor. If given, then every thin'th sample is retained (e.g., if thin is 10 then we keep samples 1, 11, 21, ...). Note that this can produce surprising results as it will always select the first sample but not necessarily always the last.

n_sample — The number of samples to draw from object *with replacement*. This means that n_sample can be larger than the total number of samples taken (though it probably should not)

pmcmc_varied_parameter *Describe varying pmcmc parameter*

Description

Describe a varying parameter for use within the nested pmcmc. Note that the name is not set here, but will end up being naturally defined when used with `pmcmc_parameters_nested`, which collects these together for use with `pmcmc()`.

Usage

```
pmcmc_varied_parameter(
  name,
  populations,
  initial,
  min = -Inf,
  max = Inf,
  discrete,
  integer = FALSE,
  prior = NULL
)
```

Arguments

`name`	Name for the parameter (a string)
`populations`	The name of the populations for which different values of the parameter are being estimated for, length `n_pop`.
`initial`	Initial value(s) for the parameter. Must be either length `n_pop` or `1`, in which case the same value is assumed for all populations.
`min`	Optional minimum value(s) for the parameter (otherwise `-Inf`). If given, then `initial` must be at least this value. Must be either length `n_pop` or `1`, in which case the same value is assumed for all populations.
`max`	Optional max value for the parameter (otherwise `Inf`). If given, then `initial` must be at most this value. Must be either length `n_pop` or `1`, in which case the same value is assumed for all populations.
`discrete`	Deprecated; use `integer` instead.
`integer`	Logical, indicating if this parameter is integer. If `TRUE` then the parameter will be rounded after a new parameter is proposed.
`prior`	A prior function (if not given an improper flat prior is used - be careful!). It must be a function that takes a single argument, being the value of this parameter. If given, then `prior(initial)` must evaluate to a finite value. Must be either length `n_pop` or `1`, in which case the same value is assumed for all populations.

Examples

```
mcstate::pmcmc_varied_parameter(
  name = "size",
  populations = c("Europe", "America"),
  initial = c(100, 200),
  min = 0,
  max = Inf,
  integer = TRUE,
  prior = list(dnorm, dexp))
```

`smc2` *Run SMC^2*

Description

Run a SMC^2. This is experimental and subject to change. Use at your own risk.

Usage

```
smc2(pars, filter, control)
```

Arguments

`pars`	A `smc2_parameters` object containing information about parameters (ranges, priors, proposal kernel, translation functions for use with the particle filter).
`filter`	A `particle_filter` object
`control`	A smc2_control object to control the behaviour of the algorithm

Value

A `smc2_result` object, with elements

- `pars`: a matrix of sampled parameters (n_parameter_set long)
- `probabilities`: a matrix of probabilities (`log_prior`, `log_likelihood`, `log_posterior` and `weight`). The latter is the log posterior normalised over all samples
- `statistics`: interesting or useful statistics about your sample, including the `ess` (effective sample size, over time), `acceptance_rate` (where a regeneration step was done, the acceptance rate), `n_particles`, `n_parameter_sets` and `n_steps` (inputs to the simulation). The `effort` field is a rough calculation of the number of particle-filter runs that this run was worth.

Examples

```
# We use an example from dust which implements an epidemiological SIR
# (Susceptible-Infected-Recovered) model; see vignette("sir_models")
# for more background, as this example follows from the pMCMC example
# there
```

```
# The key tuning here is the number of particles per filter and number
# of parameter sets to consider simultaneously. Ordinarily these would
# be set (much) higher with an increase in computing time
n_particles <- 42
n_parameter_sets <- 20

# Basic epidemiological (Susceptible-Infected-Recovered) model
sir <- dust::dust_example("sir")

# Pre-computed incidence data
incidence <- read.csv(system.file("sir_incidence.csv", package = "mcstate"))

# Annotate the data so that it is suitable for the particle filter to use
dat <- mcstate::particle_filter_data(incidence, "day", 4, 0)

# Subset the output during run
index <- function(info) {
  list(run = 5L)
}

# The comparison function, used to compare simulated data with observe
# data, given the above subset
compare <- function(state, observed, pars) {
  exp_noise <- 1e6
  incidence_modelled <- state[1L, , drop = TRUE]
  incidence_observed <- observed$cases
  lambda <- incidence_modelled +
    rexp(n = length(incidence_modelled), rate = exp_noise)
  dpois(x = incidence_observed, lambda = lambda, log = TRUE)
}

# Finally, construct the particle filter:
filter <- mcstate::particle_filter$new(dat, sir, n_particles, compare,
                                       index = index)

# To control the smc2 we need to specify the parameters to consider
pars <- mcstate::smc2_parameters$new(
  list(
    mcstate::smc2_parameter("beta",
                            function(n) runif(n, 0, 1),
                            function(x) dunif(x, 0, 1, log = TRUE),
                            min = 0, max = 1),
    mcstate::smc2_parameter("gamma",
                            function(n) runif(n, 0, 1),
                            function(x) dunif(x, 0, 1, log = TRUE),
                            min = 0, max = 1)))
control <- mcstate::smc2_control(n_parameter_sets, progress = TRUE)

# Then we run the particle filter
res <- mcstate::smc2(pars, filter, control)

# This returns quite a lot of information about the fit, and this will
# change in future versions
```

```
res

# Most useful is likely the predict method:
predict(res)
```

`smc2_control` *Control for SMC2*

Description

Control for smc2. This function constructs a list of options and does some basic validation to ensure that the options will work well together. Do not manually change the values in this object. Do not refer to any argument except `n_parameter_sets` by position as the order of the arguments may change in future.

Usage

```
smc2_control(
  n_parameter_sets,
  degeneracy_threshold = 0.5,
  covariance_scaling = 0.5,
  progress = TRUE,
  save_trajectories = FALSE
)
```

Arguments

`n_parameter_sets`
: The number of replicate parameter sets to simulate at once.

`degeneracy_threshold`
: The degeneracy threshold. Once the effective sample size drops below `degeneracy_threshold * n_parameter_sets` the algorithm will rerun simulations from the beginning of the data and use these to replenish the particles.

`covariance_scaling`
: A scaling factor to update variance covariance matrix of sampled parameters by

`progress`
: Logical, indicating if a progress bar should be displayed, using `progress::progress_bar`.

`save_trajectories`
: Logical, indicating if particle trajectories should be saved during the simulation.

Value

A `smc2_control` object, which should not be modified once created.

Examples

```
mcstate::smc2_control(100)
```

`smc2_parameter` *Describe single pmcmc parameter*

Description

Describe a single parameter for use within the SMC^2. Note that the name is not set here, but will end up being naturally defined when used with `smc2_parameters`, which collects these together for use with `smc2()`.

Usage

```
smc2_parameter(
  name,
  sample,
  prior,
  min = -Inf,
  max = Inf,
  discrete,
  integer = FALSE
)
```

Arguments

`name`	Name for the parameter (a string)
`sample`	A sampling function; it must take a single argument representing the number of sampled to be returned. Typically this will be a `r` probability function corresponding to the sampling version of your prior (e.g., you might use `runif` and `dunif` for `sample` and `prior`). If you provide `min`, `max` or `integer` you *must* ensure that your function returns values that satisfy these constraints, as this is not (yet) checked.
`prior`	A prior function. It must be a function that takes a single argument, being the value of this parameter.
`min`	Optional minimum value for the parameter (otherwise `-Inf`). If given, then `initial` must be at least this value.
`max`	Optional max value for the parameter (otherwise `Inf`). If given, then `initial` must be at most this value.
`discrete`	Deprecated; use `integer` instead.
`integer`	Logical, indicating if this parameter is an integer. If `TRUE` then the parameter will be rounded after a new parameter is proposed.

Examples

```
mcstate::smc2_parameter("a",
                        function(n) rnorm(n),
                        function(x) dnorm(n, log = TRUE))
```

smc2_parameters *smc2_parameters*

Description

Construct parameters for use with smc2(). This creates a utility object that is used internally to work with parameters. Most users only need to construct this object, but see the examples for how it can be used.

Methods

Public methods:

- smc2_parameters$new()
- smc2_parameters$sample()
- smc2_parameters$names()
- smc2_parameters$summary()
- smc2_parameters$prior()
- smc2_parameters$propose()
- smc2_parameters$model()

Method new(): Create the smc2_parameters object

Usage:

```
smc2_parameters$new(parameters, transform = NULL)
```

Arguments:

parameters A list of smc2_parameter objects, each of which describe a single parameter in your model. If parameters is named, then these names must match the $name element of each parameter is used (this is verified).

transform An optional transformation function to apply to your parameter vector immediately before passing it to the model function. If not given, then as.list is used, as dust models require this. However, if t you need to generate derived parameters from those being actively sampled you can do arbitrary transformations here.

Method sample(): Create n independent random parameter vectors (as a matrix with n rows)

Usage:

```
smc2_parameters$sample(n)
```

Arguments:

n Number of replicate parameter sets to draw

Method names(): Return the names of the parameters

Usage:

```
smc2_parameters$names()
```

Method summary(): Return a data.frame with information about parameters (name, min, max, and integer).

Usage:

```
smc2_parameters$summary()
```

Method `prior()`**:** Compute the prior for a parameter vector

Usage:

```
smc2_parameters$prior(theta)
```

Arguments:

`theta` a parameter vector in the same order as your parameters were defined in (see `$names()` for that order.

Method `propose()`**:** Propose a new parameter vector given a current parameter vector and variance covariance matrix. After proposal, this rounds any integer values, and reflects bounded parameters until they lie within `min`:`max`.

Usage:

```
smc2_parameters$propose(theta, vcv)
```

Arguments:

`theta` a parameter vector in the same order as your parameters were defined in (see `$names()` for that order).

`vcv` the variance covariance matrix for the proposal; must be square and have a number of rows and columns equal to the number of parameters, in the same order as `theta`.

Method `model()`**:** Apply the model transformation function to a parameter vector.

Usage:

```
smc2_parameters$model(theta)
```

Arguments:

`theta` a parameter vector in the same order as your parameters were defined in (see `$names()` for that order.

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