

Package ‘optimizeR’

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Title Unified Framework for Numerical Optimizers

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Description Provides a unified object-oriented framework for numerical optimizers in R. Allows for both minimization and maximization with any optimizer, optimization over more than one function argument, measuring of computation time, setting a time limit for long optimization tasks.

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|-----------|--|
| Objective | <i>Specify objective function object</i> |
|-----------|--|

Description

The `Objective` object specifies the framework for an objective function for numerical optimization.

Value

An `Objective` object.

Active bindings

`objective_name` [character(1)]
The label for the objective function.

`fixed_arguments` [character()]
The name(s) of the fixed argument(s) (if any).

`seconds` [numeric(1)]
A time limit in seconds. Computations are interrupted prematurely if `seconds` is exceeded.
No time limit if `seconds = Inf` (the default).
Note the limitations documented in [setTimeLimit](#).

`hide_warnings` [logical(1)]
Hide warnings when evaluating the objective function?

`verbose` [logical(1)]
Print status messages?

`npar` [integer()]
The length of each target argument.

`target` [character()]
The argument name(s) that get optimized.

`gradient_specified` [logical(1)]
Whether a gradient function has been specified via `$set_gradient()`.

`hessian_specified` [logical(1)]
Whether a Hessian function has been specified via `$set_hessian()`.

Methods**Public methods:**

- [Objective\\$new\(\)](#)
- [Objective\\$set_argument\(\)](#)
- [Objective\\$get_argument\(\)](#)
- [Objective\\$remove_argument\(\)](#)
- [Objective\\$set_gradient\(\)](#)

- `Objective$set_hessian()`
- `Objective$evaluate()`
- `Objective$evaluate_gradient()`
- `Objective$evaluate_hessian()`
- `Objective$print()`
- `Objective$clone()`

Method `new()`: Creates a new Objective object.

Usage:

```
Objective$new(f, target = NULL, npar, ...)
```

Arguments:

`f` [function]

A function to be optimized.

It is expected that `f` has at least one numeric argument.

Further, it is expected that the return value of `f` is of the structure `numeric(1)`, i.e. a single numeric value.

`target` [character()]

The argument name(s) that get optimized.

All target arguments must be numeric.

Can be NULL (default), then the first function argument is selected.

`npar` [integer()]

The length of each target argument, i.e., the length(s) of the numeric vector argument(s) specified by `target`.

... Optionally additional function arguments that are fixed during the optimization.

Method `set_argument()`: Set a function argument that remains fixed during optimization.

Usage:

```
Objective$set_argument(..., .overwrite = TRUE, .verbose = self$verbose)
```

Arguments:

... Optionally additional function arguments that are fixed during the optimization.

`.overwrite` [logical(1)]

Overwrite existing values?

`.verbose` [logical(1)]

Print status messages?

Method `get_argument()`: Get a fixed function argument.

Usage:

```
Objective$get_argument(argument_name, .verbose = self$verbose)
```

Arguments:

`argument_name` [character(1)]

A function argument name.

`.verbose` [logical(1)]

Print status messages?

Method `remove_argument()`: Remove a fixed function argument.

Usage:

```
Objective$remove_argument(argument_name, .verbose = self$verbose)
```

Arguments:

```
argument_name [character(1)]
```

A function argument name.

```
.verbose [logical(1)]
```

Print status messages?

Method `set_gradient()`: Set a gradient function.

Usage:

```
Objective$set_gradient(
  gradient,
  target = self$target,
  npar = self$npar,
  ...,
  .verbose = self$verbose
)
```

Arguments:

```
gradient [function]
```

A function that computes the gradient of the objective function *f*.

It is expected that `gradient` has the same call as *f*, and that `gradient` returns a numeric vector of length `self$npar`.

```
target [character()]
```

The argument name(s) that get optimized.

All target arguments must be numeric.

Can be NULL (default), then the first function argument is selected.

```
npar [integer()]
```

The length of each target argument, i.e., the length(s) of the numeric vector argument(s) specified by `target`.

... Optionally additional function arguments that are fixed during the optimization.

```
.verbose [logical(1)]
```

Print status messages?

Method `set_hessian()`: Set a Hessian function.

Usage:

```
Objective$set_hessian(
  hessian,
  target = self$target,
  npar = self$npar,
  ...,
  .verbose = self$verbose
)
```

Arguments:

```
hessian [function]
```

A function that computes the Hessian of the objective function *f*.

It is expected that `hessian` has the same call as *f*, and that `hessian` returns a numeric matrix of dimension `self$npar` times `self$npar`.

target [character()]
 The argument name(s) that get optimized.
 All target arguments must be numeric.
 Can be NULL (default), then the first function argument is selected.

npar [integer()]
 The length of each target argument, i.e., the length(s) of the numeric vector argument(s) specified by target.

... Optionally additional function arguments that are fixed during the optimization.

.verbose [logical(1)]
 Print status messages?

Method evaluate(): Evaluate the objective function.

Usage:

```
Objective$evaluate(
  .at,
  .negate = FALSE,
  .gradient_as_attribute = FALSE,
  .gradient_attribute_name = "gradient",
  .hessian_as_attribute = FALSE,
  .hessian_attribute_name = "hessian",
  ...
)
```

Arguments:

.at [numeric()]
 The values for the target argument(s), written in a single vector. (Must be of length sum(self\$npar).)

.negate [logical(1)]
 Negate the function return value?

.gradient_as_attribute [logical(1)]
 Add the value of the gradient function as an attribute to the output?
 The attribute name is defined via the .gradient_attribute_name argument.
 Ignored if \$gradient_specified is FALSE.

.gradient_attribute_name [character(1)]\cr Only relevant if .gradient_as_attribute = TRUE:
 In that case, the attribute name for the gradient (if available).

.hessian_as_attribute [logical(1)]
 Add the value of the Hessian function as an attribute to the output?
 The attribute name is defined via the .hessian_attribute_name argument.
 Ignored if \$hessian_specified is FALSE.

.hessian_attribute_name [character(1)]\cr Only relevant if .hessian_as_attribute = TRUE:
 In that case, the attribute name for the Hessian (if available).

... Optionally additional function arguments that are fixed during the optimization.

Method evaluate_gradient(): Evaluate the gradient function.

Usage:

```
Objective$evaluate_gradient(.at, .negate = FALSE, ...)
```

Arguments:

```
.at [numeric()]
```

The values for the target argument(s), written in a single vector. (Must be of length `sum(self$npar)`.)

```
.negate [logical(1)]
```

Negate the function return value?

... Optionally additional function arguments that are fixed during the optimization.

Method `evaluate_hessian()`: Evaluate the Hessian function.

Usage:

```
Objective$evaluate_hessian(.at, .negate = FALSE, ...)
```

Arguments:

```
.at [numeric()]
```

The values for the target argument(s), written in a single vector. (Must be of length `sum(self$npar)`.)

```
.negate [logical(1)]
```

Negate the function return value?

... Optionally additional function arguments that are fixed during the optimization.

Method `print()`: Print details of the Objective object.

Usage:

```
Objective$print()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
Objective$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
### define log-likelihood function of Gaussian mixture model
llk <- function(mu, sd, lambda, data) {
  sd <- exp(sd)
  lambda <- plogis(lambda)
  cluster_1 <- lambda * dnorm(data, mu[1], sd[1])
  cluster_2 <- (1 - lambda) * dnorm(data, mu[2], sd[2])
  sum(log(cluster_1 + cluster_2))
}

### optimize over the first three arguments, the 'data' argument is constant
objective <- Objective$new(
  f = llk, target = c("mu", "sd", "lambda"), npar = c(2, 2, 1),
  data = faithful$eruptions
)

### evaluate at 1:5 (1:2 is passed to mu, 3:4 to sd, and 5 to lambda)
objective$evaluate(1:5)
```

Optimizer

Specify numerical optimizer object

Description

The `Optimizer` object defines a numerical optimizer based on any optimization algorithm implemented in R. The main advantage of working with an `Optimizer` object instead of using the optimization function directly lies in the standardized inputs and outputs.

Any R function that fulfills the following four constraints can be defined as an `Optimizer` object:

1. It must have an input for a function, the objective function to be optimized.
2. It must have an input for a numeric vector, the initial values from where the optimizer starts.
3. It must have a `...` argument for additional parameters passed on to the objective function.
4. The output must be a named list, including the optimal function value and the optimal parameter vector.

Active bindings

`label` [character(1)]

The label for the optimizer.

`algorithm` [function]

The optimization algorithm.

`arg_objective` [character(1)]

The argument name for the objective function in `algorithm`.

`arg_initial` [character(1)]

The argument name for the initial values in `algorithm`.

`arg_lower` [character(1) | NA]

Optionally the argument name for the lower parameter bound in `algorithm`.

Can be NA if not available.

`arg_upper` [character(1) | NA]

Optionally the argument name for the upper parameter bound in `algorithm`.

Can be NA if not available.

`arg_gradient` [character(1) | NA]

Optionally the argument name for the gradient function in `algorithm`.

Can be NA if not available.

`arg_hessian` [character(1) | NA]

Optionally the argument name for the Hessian function in `algorithm`.

Can be NA if not available.

`gradient_as_attribute` [logical(1)]

Only relevant if `arg_gradient` is not NA.

In that case, does `algorithm` expect that the gradient is an attribute of the objective function output (as for example in `nlm`)? In that case, `arg_gradient` defines the attribute name.

`hessian_as_attribute` [logical(1)]
 Only relevant if `arg_hessian` is not NA.
 In that case, does algorithm expect that the Hessian is an attribute of the objective function output (as for example in `nlm`)? In that case, `arg_hessian` defines the attribute name.

`out_value` [character(1)]
 The element name for the optimal function value in the output list of algorithm.

`out_parameter` [character(1)]
 The element name for the optimal parameters in the output list of algorithm.

`direction` [character(1)]
 Either "min" (if the optimizer minimizes) or "max" (if the optimizer maximizes).

`arguments` [list()]
 Custom arguments for algorithm.
 Defaults are used for arguments that are not specified.

`seconds` [numeric(1)]
 A time limit in seconds.
 Optimization is interrupted prematurely if seconds is exceeded.
 No time limit if seconds = Inf (the default).
 Note the limitations documented in `setTimeLimit`.

`hide_warnings` [logical(1)]
 Hide warnings during optimization?

`output_ignore` [character()]
 Elements to ignore (not include) in the optimization output.

Methods

Public methods:

- `Optimizer$new()`
- `Optimizer$definition()`
- `Optimizer$set_arguments()`
- `Optimizer$minimize()`
- `Optimizer$maximize()`
- `Optimizer$optimize()`
- `Optimizer$print()`
- `Optimizer$clone()`

Method `new()`: Initializes a new Optimizer object.

Usage:

```
Optimizer$new(which, ..., .verbose = TRUE)
```

Arguments:

`which` [character(1)]

Either:

- one of `optimizer_dictionary$keys`
- or "custom", in which case `$definition()` must be used to define the optimizer details.

... [any]
 Optionally additional named arguments to be passed to the optimizer algorithm. Without specifications, default values of the optimizer are used.

.verbose [logical(1)]
 Print status messages?

Returns: A new Optimizer object.

Method definition(): Defines an optimizer.

Usage:

```
Optimizer$definition(
  algorithm,
  arg_objective,
  arg_initial,
  arg_lower = NA,
  arg_upper = NA,
  arg_gradient = NA,
  arg_hessian = NA,
  gradient_as_attribute = FALSE,
  hessian_as_attribute = FALSE,
  out_value,
  out_parameter,
  direction
)
```

Arguments:

algorithm [function]
 The optimization algorithm.

arg_objective [character(1)]
 The argument name for the objective function in algorithm.

arg_initial [character(1)]
 The argument name for the initial values in algorithm.

arg_lower [character(1) | NA]
 Optionally the argument name for the lower parameter bound in algorithm.
 Can be NA if not available.

arg_upper [character(1) | NA]
 Optionally the argument name for the upper parameter bound in algorithm.
 Can be NA if not available.

arg_gradient [character(1) | NA]
 Optionally the argument name for the gradient function in algorithm.
 Can be NA if not available.

arg_hessian [character(1) | NA]
 Optionally the argument name for the Hessian function in algorithm.
 Can be NA if not available.

gradient_as_attribute [logical(1)]
 Only relevant if arg_gradient is not NA.
 In that case, does algorithm expect that the gradient is an attribute of the objective function output (as for example in `nlm`)? In that case, arg_gradient defines the attribute name.

`hessian_as_attribute` [logical(1)]

Only relevant if `arg_hessian` is not NA.

In that case, does `algorithm` expect that the Hessian is an attribute of the objective function output (as for example in `nlm`)? In that case, `arg_hessian` defines the attribute name.

`out_value` [character(1)]

The element name for the optimal function value in the output list of `algorithm`.

`out_parameter` [character(1)]

The element name for the optimal parameters in the output list of `algorithm`.

`direction` [character(1)]

Either "min" (if the optimizer minimizes) or "max" (if the optimizer maximizes).

Method `set_arguments()`: Sets optimizer arguments.

Usage:

```
Optimizer$set_arguments(...)
```

Arguments:

... [any]

Optionally additional named arguments to be passed to the optimizer algorithm. Without specifications, default values of the optimizer are used.

Returns: The Optimizer object.

Method `minimize()`: Performing minimization.

Usage:

```
Optimizer$minimize(objective, initial, lower = NA, upper = NA, ...)
```

Arguments:

`objective` [function|Objective]

A function to be optimized that

1. has at least one argument that receives a numeric vector
2. and returns a single numeric value.

Alternatively, it can also be an [Objective](#) object for more flexibility.

`initial` [numeric()]

Starting parameter values for the optimization.

`lower` [NA|numeric()|numeric(1)]

Lower bounds on the parameters.

If a single number, this will be applied to all parameters.

Can be NA to not define any bounds.

`upper` [NA|numeric()|numeric(1)]

Upper bounds on the parameters.

If a single number, this will be applied to all parameters.

Can be NA to not define any bounds.

... [any]

Optionally additional named arguments to be passed to the optimizer algorithm. Without specifications, default values of the optimizer are used.

Returns: A named list, containing at least these five elements:

`value` A numeric, the minimum function value.

parameter A numeric vector, the parameter vector where the minimum is obtained.
seconds A numeric, the optimization time in seconds.
initial A numeric, the initial parameter values.
error Either TRUE if an error occurred, or FALSE, else.
Appended are additional output elements of the optimizer.
If an error occurred, then the error message is also appended as element `error_message`.
If the time limit was exceeded, this counts as an error. In addition, the flag `time_out = TRUE` is appended.

Examples:

```
Optimizer$new("stats::nlm")$
  minimize(objective = function(x) x^4 + 3*x - 5, initial = 2)
```

Method `maximize()`: Performing maximization.

Usage:

```
Optimizer$maximize(objective, initial, lower = NA, upper = NA, ...)
```

Arguments:

`objective` [function|Objective]

A function to be optimized that

1. has at least one argument that receives a numeric vector
2. and returns a single numeric value.

Alternatively, it can also be an [Objective](#) object for more flexibility.

`initial` [numeric()]

Starting parameter values for the optimization.

`lower` [NA|numeric()|numeric(1)]

Lower bounds on the parameters.

If a single number, this will be applied to all parameters.

Can be NA to not define any bounds.

`upper` [NA|numeric()|numeric(1)]

Upper bounds on the parameters.

If a single number, this will be applied to all parameters.

Can be NA to not define any bounds.

`...` [any]

Optionally additional named arguments to be passed to the optimizer algorithm. Without specifications, default values of the optimizer are used.

Returns: A named list, containing at least these five elements:

`value` A numeric, the maximum function value.

`parameter` A numeric vector, the parameter vector where the maximum is obtained.

`seconds` A numeric, the optimization time in seconds.

`initial` A numeric, the initial parameter values.

`error` Either TRUE if an error occurred, or FALSE, else.

Appended are additional output elements of the optimizer.

If an error occurred, then the error message is also appended as element `error_message`.

If the time limit was exceeded, this also counts as an error. In addition, the flag `time_out = TRUE` is appended.

Examples:

```
Optimizer$new("stats::nlm")$
  maximize(objective = function(x) -x^4 + 3*x - 5, initial = 2)
```

Method `optimize()`: Performing minimization or maximization.

Usage:

```
Optimizer$optimize(
  objective,
  initial,
  lower = NA,
  upper = NA,
  direction = "min",
  ...
)
```

Arguments:

`objective` [function|Objective]

A function to be optimized that

1. has at least one argument that receives a numeric vector
2. and returns a single numeric value.

Alternatively, it can also be an [Objective](#) object for more flexibility.

`initial` [numeric()]

Starting parameter values for the optimization.

`lower` [NA|numeric()|numeric(1)]

Lower bounds on the parameters.

If a single number, this will be applied to all parameters.

Can be NA to not define any bounds.

`upper` [NA|numeric()|numeric(1)]

Upper bounds on the parameters.

If a single number, this will be applied to all parameters.

Can be NA to not define any bounds.

`direction` [character(1)]

Either "min" for minimization or "max" for maximization.

`...` [any]

Optionally additional named arguments to be passed to the optimizer algorithm. Without specifications, default values of the optimizer are used.

Returns: A named list, containing at least these five elements:

`value` A numeric, the maximum function value.

`parameter` A numeric vector, the parameter vector where the maximum is obtained.

`seconds` A numeric, the optimization time in seconds.

`initial` A numeric, the initial parameter values.

`error` Either TRUE if an error occurred, or FALSE, else.

Appended are additional output elements of the optimizer.

If an error occurred, then the error message is also appended as element `error_message`.

If the time limit was exceeded, this also counts as an error. In addition, the flag `time_out = TRUE` is appended.

Examples:

```
objective <- function(x) -x^4 + 3*x - 5
optimizer <- Optimizer$new("stats::nlm")
optimizer$optimize(objective = objective, initial = 2, direction = "min")
optimizer$optimize(objective = objective, initial = 2, direction = "max")
```

Method `print()`: Prints the optimizer label.

Usage:

```
Optimizer$print(...)
```

Arguments:

```
... [any]
```

Optionally additional named arguments to be passed to the optimizer algorithm. Without specifications, default values of the optimizer are used.

Returns: Invisibly the Optimizer object.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
Optimizer$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
### Task: compare minimization with 'stats::nlm' and 'pracma::nelder_mead'

# 1. define objective function and initial values
objective <- TestFunctions::TF_ackley
initial <- c(3, 3)

# 2. get overview of optimizers available in dictionary
optimizer_dictionary$keys

# 3. define 'nlm' optimizer
nlm <- Optimizer$new(which = "stats::nlm")

# 4. define the 'pracma::nelder_mead' optimizer (not contained in the dictionary)
nelder_mead <- Optimizer$new(which = "custom")
nelder_mead$definition(
  algorithm = pracma::nelder_mead, # the optimization function
  arg_objective = "fn",           # the argument name for the objective function
  arg_initial = "x0",            # the argument name for the initial values
  out_value = "fmin",           # the element for the optimal function value in the output
  out_parameter = "xmin",       # the element for the optimal parameters in the output
  direction = "min"             # the optimizer minimizes
)

# 5. compare the minimization results
nlm$minimize(objective, initial)
nelder_mead$minimize(objective, initial)
```

```

## -----
## Method `Optimizer$minimize`
## -----

Optimizer$new("stats::nlm")$
  minimize(objective = function(x) x^4 + 3*x - 5, initial = 2)

## -----
## Method `Optimizer$maximize`
## -----

Optimizer$new("stats::nlm")$
  maximize(objective = function(x) -x^4 + 3*x - 5, initial = 2)

## -----
## Method `Optimizer$optimize`
## -----

objective <- function(x) -x^4 + 3*x - 5
optimizer <- Optimizer$new("stats::nlm")
optimizer$optimize(objective = objective, initial = 2, direction = "min")
optimizer$optimize(objective = objective, initial = 2, direction = "max")

```

optimizer_dictionary *Dictionary of optimizer functions*

Description

A dictionary of currently included numerical optimizer functions in the {optimizer} package.

Usage

```
optimizer_dictionary
```

Format

An R6 object of class [Dictionary](#).

Examples

```
print(optimizer_dictionary)
```

| | |
|-----------------|--|
| ParameterSpaces | <i>Switch between parameter spaces</i> |
|-----------------|--|

Description

The ParameterSpaces object manages two related parameter spaces:

- the Optimization Space (for optimization)
- and the Interpretation Space (for easier interpretation).

In the Optimization Space, parameters are stored as a numeric vector, the standard format for numerical optimizers.

In the Interpretation Space, parameters are stored as a list and can take different formats (e.g., matrix).

The user can define transformation functions (not necessarily bijective) to switch between these spaces via the `$o2i()` and `$i2o()` methods.

Methods

Public methods:

- `ParameterSpaces$new()`
- `ParameterSpaces$print()`
- `ParameterSpaces$switch()`
- `ParameterSpaces$o2i()`
- `ParameterSpaces$i2o()`
- `ParameterSpaces$clone()`

Method `new()`: Initializes a new ParameterSpaces object.

Usage:

```
ParameterSpaces$new(parameter_names, parameter_lengths_in_o_space)
```

Arguments:

`parameter_names` [character()]

Unique names for the parameters.

`parameter_lengths_in_o_space` [integer()]

The length of each parameter in the optimization space.

Returns: A new ParameterSpaces object.

Method `print()`: Print an overview of the parameter spaces.

Usage:

```
ParameterSpaces$print(show_transformer = FALSE)
```

Arguments:

`show_transformer` [logical(1)]

Show transformer functions in the output?

Method `switch()`: Switch between Optimization Space and Interpretation Space.

Usage:

```
ParameterSpaces$switch(x, to = NULL)
```

Arguments:

`x` [numeric() | list()]

The parameters, either as a numeric vector (will be switched to Interpretation Space), or as a list() (will be switched to Optimization Space).

`to` [character(1) | NULL]

Explicitly switch to a specific space, either

- "o": Optimization Space
- "i": Interpretation Space

If NULL, the function will switch to the other space.

Method `o2i()`: Define transformation functions when switching from Optimization Space to Interpretation Space.

Usage:

```
ParameterSpaces$o2i(...)
```

Arguments:

... [function]

One or more transformation functions, named according to the parameters.

Transformers from Optimization Space to Interpretation Space (`o2i`) **must receive** a numeric.

The default is the identity.

Method `i2o()`: Define transformation functions when switching from Interpretation Space to Optimization Space.

Usage:

```
ParameterSpaces$i2o(...)
```

Arguments:

... [function]

One or more transformers functions, named according to the parameters.

Transformers from Interpretation Space to Optimization Space (`i2o`) **must return** a numeric.

The default is `as.vector()`.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
ParameterSpaces$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
### Log-likelihood function of two-class Gaussian mixture model with
### parameter vector `theta` that consists of
### - `mu`, mean vector of length 2
### - `sd`, standard deviation vector of length 2, must be positive
```



```

### - `lambda`, class probability of length 1, must be between 0 and 1

normal_mixture_llk <- function(theta, data) {
  mu <- theta[1:2]
  sd <- exp(theta[3:4])
  lambda <- plogis(theta[5])
  c1 <- lambda * dnorm(data, mu[1], sd[1])
  c2 <- (1 - lambda) * dnorm(data, mu[2], sd[2])
  sum(log(c1 + c2))
}

### define parameter spaces
### - `mu` needs no transformation
### - `sd` needs to be real in optimization space and positive in
###   interpretation space
### - `lambda` needs to be real and of length `1` in optimization space, and
###   a probability vector of length `2` in interpretation space

normal_mixture_spaces <- ParameterSpaces$
  new(
    parameter_names = c("mu", "sd", "lambda"),
    parameter_lengths_in_o_space = c(2, 2, 1)
  )$
  o2i(
    "mu" = function(x) x,
    "sd" = function(x) exp(x),
    "lambda" = function(x) c(plogis(x), 1 - plogis(x))
  )$
  i2o(
    "mu" = function(x) x,
    "sd" = function(x) log(x),
    "lambda" = function(x) qlogis(x[1])
  )

### switch between parameter spaces

par <- list(
  "mu" = c(2, 4),
  "sd" = c(0.5, 1),
  "lambda" = c(0.4, 0.6)
)
(x <- normal_mixture_spaces$switch(par)) # switch to optimization space
normal_mixture_llk(
  theta = x, data = datasets::faithful$eruptions
)
normal_mixture_spaces$switch(x) # switch back

```

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