

Package ‘ao’

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Title Alternating Optimization

Version 1.2.1

Description An iterative process that optimizes a function by alternately performing restricted optimization over parameter subsets. Instead of joint optimization, it breaks the optimization problem down into simpler sub-problems. This approach can make optimization feasible when joint optimization is too difficult.

URL <https://loelschlaeger.de/ao/>, <https://github.com/loelschlaeger/ao/>

BugReports <https://github.com/loelschlaeger/ao/issues>

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ao	<i>Alternating Optimization</i>
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Description

Alternating optimization (AO) is an iterative process for optimizing a real-valued function jointly over all its parameters by alternating restricted optimization over parameter partitions.

Usage

```
ao(
  f,
  initial,
  target = NULL,
  npar = NULL,
  gradient = NULL,
  hessian = NULL,
  ...,
  partition = "sequential",
  new_block_probability = 0.3,
  minimum_block_number = 1,
  minimize = TRUE,
  lower = NULL,
  upper = NULL,
  iteration_limit = Inf,
  seconds_limit = Inf,
  tolerance_value = 1e-06,
  tolerance_parameter = 1e-06,
  tolerance_parameter_norm = function(x, y) sqrt(sum((x - y)^2)),
  tolerance_history = 1,
  base_optimizer = Optimizer$new("stats::optim", method = "L-BFGS-B"),
  verbose = FALSE,
  hide_warnings = TRUE,
  add_details = TRUE
)
```

Arguments

f	[function] A function to be optimized, returning a single numeric value. The first argument of f should be a numeric of the same length as initial, optionally followed by any other arguments specified by the ... argument. If f is to be optimized over an argument other than the first, or more than one argument, this has to be specified via the target argument.
---	--

initial	[numeric() list()] The starting parameter values for the target argument(s). This can also be a list of multiple starting parameter values, see details.
target	[character() NULL] The name(s) of the argument(s) over which <code>f</code> gets optimized. This can only be numeric arguments. Can be NULL (default), then it is the first argument of <code>f</code>.
npar	[integer()] The length(s) of the target argument(s). Must be specified if more than two target arguments are specified via the <code>target</code> argument. Can be NULL if there is only one target argument, in which case <code>npar</code> is set to be <code>length(initial)</code>.
gradient	[function NULL] Optionally a function that returns the gradient of <code>f</code>. The function call of <code>gradient</code> must be identical to <code>f</code>. Ignored if <code>base_optimizer</code> does not support custom gradient.
hessian	[function NULL] Optionally a function that returns the Hessian of <code>f</code>. The function call of <code>hessian</code> must be identical to <code>f</code>. Ignored if <code>base_optimizer</code> does not support custom Hessian.
...	Additional arguments to be passed to <code>f</code> (and <code>gradient</code>).
partition	[character(1) list()] Defines the parameter partition, and can be either • "sequential" for treating each parameter separately, • "random" for a random partition in each iteration, • "none" for no partition (which is equivalent to joint optimization), • or a list of vectors of parameter indices, specifying a custom partition for the AO process. This can also be a list of multiple partition definitions, see details.
new_block_probability	[numeric(1)] Only relevant if <code>partition = "random"</code>. The probability for a new parameter block when creating a random partition. Values close to 0 result in larger parameter blocks, values close to 1 result in smaller parameter blocks.
minimum_block_number	[integer(1)] Only relevant if <code>partition = "random"</code>. The minimum number of blocks in random partitions.
minimize	[logical(1)] Minimize during the AO process? If FALSE, maximization is performed.

lower, upper	[numeric() NULL] Optionally lower and upper parameter bounds. Ignored if base_optimizer does not support parameter bounds.
iteration_limit	[integer(1) Inf] The maximum number of iterations through the parameter partition before the AO process is terminated. Can also be Inf for no iteration limit.
seconds_limit	[numeric(1)] The time limit in seconds before the AO process is terminated. Can also be Inf for no time limit. Note that this stopping criteria is only checked <i>after</i> a sub-problem is solved and not <i>within</i> solving a sub-problem, so the actual process time can exceed this limit.
tolerance_value	[numeric(1)] A non-negative tolerance value. The AO process terminates if the absolute difference between the current function value and the one before tolerance_history iterations is smaller than tolerance_value. Can be 0 for no value threshold.
tolerance_parameter	[numeric(1)] A non-negative tolerance value. The AO process terminates if the distance between the current estimate and the before tolerance_history iterations is smaller than tolerance_parameter. Can be 0 for no parameter threshold. By default, the distance is measured using the euclidean norm, but another norm can be specified via the tolerance_parameter_norm argument.
tolerance_parameter_norm	[function] The norm that measures the distance between the current estimate and the one from the last iteration. If the distance is smaller than tolerance_parameter, the AO process is terminated. It must be of the form function(x, y) for two vector inputs x and y, and return a single numeric value. By default, the euclidean norm function(x, y) sqrt(sum((x - y)^2)) is used.
tolerance_history	[integer(1)] The number of iterations to look back to determine whether tolerance_value or tolerance_parameter has been reached.
base_optimizer	[Optimizer list()] An Optimizer object, which can be created via Optimizer. It numerically solves the sub-problems. By default, the optim optimizer with method = "L-BFGS-B" is used. This can also be a list of multiple base optimizers, see details.

verbose	[logical(1)] Print tracing details during the AO process? Not supported when using multiple processes, see details.
hide_warnings	[logical(1)] Hide warnings during the AO process?
add_details	[logical(1)] Add details about the AO process to the output?

Details

Multiple processes:

AO can suffer from local optima. To increase the likelihood of reaching the global optimum, you can specify:

- multiple starting parameters
- multiple parameter partitions
- multiple base optimizers

Use the `initial`, `partition`, and/or `base_optimizer` arguments to provide a list of possible values for each parameter. Each combination of initial values, parameter partitions, and base optimizers will create a separate AO process.

Output value:

In the case of multiple processes, the output values refer to the optimal (with respect to function value) AO processes.

If `add_details = TRUE`, the following elements are added:

- `estimates` is a list of optimal parameters in each process.
- `values` is a list of optimal function values in each process.
- `details` combines details of the single processes and has an additional column process with an index for the different processes.
- `seconds_each` gives the computation time in seconds for each process.
- `stopping_reasons` gives the termination message for each process.
- `processes` give details how the different processes were specified.

Parallel computation:

By default, processes run sequentially. However, since they are independent, they can be parallelized. To enable parallel computation, use the `{future}` framework. For example, run the following *before* the `ao()` call:

```
future::plan(future::multisession, workers = 4)
```

Progress updates:

When using multiple processes, setting `verbose = TRUE` to print tracing details during AO is not supported. However, you can still track the progress using the `{progressr}` framework. For example, run the following *before* the `ao()` call:

```
progressr::handlers(global = TRUE)
progressr::handlers(
  progressr::handler_progress(":percent :eta :message")
)
```

Value

A list with the following elements:

- `estimate` is the parameter vector at termination.
- `value` is the function value at termination.
- `details` is a data.frame with information about the AO process: For each iteration (column iteration) it contains the function value (column value), parameter values (columns starting with `p` followed by the parameter index), the active parameter block (columns starting with `b` followed by the parameter index, where 1 stands for a parameter contained in the active parameter block and 0 if not), and computation times in seconds (column seconds). Only available if `add_details = TRUE`.
- `seconds` is the overall computation time in seconds.
- `stopping_reason` is a message why the AO process has terminated.

In the case of multiple processes, the output changes slightly, see details.

Examples

```
# Example 1: Minimization of Himmelblau's function -----
himmelblau <- function(x) (x[1]^2 + x[2] - 11)^2 + (x[1] + x[2]^2 - 7)^2
ao(f = himmelblau, initial = c(0, 0))

# Example 2: Maximization of 2-class Gaussian mixture log-likelihood -----

# target arguments:
# - class means mu (2, unrestricted)
# - class standard deviations sd (2, must be non-negative)
# - class proportion lambda (only 1 for identification, must be in [0, 1])

normal_mixture_llk <- function(mu, sd, lambda, data) {
  c1 <- lambda * dnorm(data, mu[1], sd[1])
  c2 <- (1 - lambda) * dnorm(data, mu[2], sd[2])
  sum(log(c1 + c2))
}

set.seed(123)

ao(
  f = normal_mixture_llk,
  initial = runif(5),
  target = c("mu", "sd", "lambda"),
  npar = c(2, 2, 1),
  data = datasets::faithful$eruptions,
  partition = list("sequential", "random", "none"),
  minimize = FALSE,
  lower = c(-Inf, -Inf, 0, 0, 0),
  upper = c(Inf, Inf, Inf, Inf, 1),
  add_details = FALSE
)
```

Process

Process Object

Description

This object specifies an AO process.

Active bindings

`npar` [integer(1)]

The (total) length of the target argument(s).

`partition` [character(1) | list()]

Defines the parameter partition, and can be either

- "sequential" for treating each parameter separately,
- "random" for a random partition in each iteration,
- "none" for no partition (which is equivalent to joint optimization),
- or a list of vectors of parameter indices, specifying a custom partition for the AO process.

`new_block_probability` [numeric(1)]

Only relevant if `partition = "random"`.

The probability for a new parameter block when creating a random partition.

Values close to 0 result in larger parameter blocks, values close to 1 result in smaller parameter blocks.

`minimum_block_number` [integer(1)]

Only relevant if `partition = "random"`.

The minimum number of blocks in random partitions.

`verbose` [logical(1)]

Print tracing details during the AO process?

`minimize` [logical(1)]

Minimize during the AO process?

If FALSE, maximization is performed.

`iteration_limit` [integer(1) | Inf]

The maximum number of iterations through the parameter partition before the AO process is terminated.

Can also be Inf for no iteration limit.

`seconds_limit` [numeric(1)]

The time limit in seconds before the AO process is terminated.

Can also be Inf for no time limit.

Note that this stopping criteria is only checked *after* a sub-problem is solved and not *within* solving a sub-problem, so the actual process time can exceed this limit.

`tolerance_value` [numeric(1)]

A non-negative tolerance value. The AO process terminates if the absolute difference between the current function value and the one before `tolerance_history` iterations is smaller than `tolerance_value`.

Can be 0 for no value threshold.

`tolerance_parameter` [numeric(1)]

A non-negative tolerance value. The AO process terminates if the distance between the current estimate and the before `tolerance_history` iterations is smaller than `tolerance_parameter`.

Can be 0 for no parameter threshold.

By default, the distance is measured using the euclidean norm, but another norm can be specified via the `tolerance_parameter_norm` field.

`tolerance_parameter_norm` [function]

The norm that measures the distance between the current estimate and the one from the last iteration. If the distance is smaller than `tolerance_parameter`, the AO process is terminated.

It must be of the form `function(x, y)` for two vector inputs `x` and `y`, and return a single numeric value. By default, the euclidean norm `function(x, y) sqrt(sum((x - y)^2))` is used.

`tolerance_history` [integer(1)]

The number of iterations to look back to determine whether `tolerance_value` or `tolerance_parameter` has been reached.

`add_details` [logical(1)]

Add details about the AO process to the output?

`iteration` [integer(1)]

The current iteration number.

`block` [integer()]

The currently active parameter block, represented as parameter indices.

`output` [list(), read-only]

The output of the AO process, which is a list with the following elements:

- `estimate` is the parameter vector at termination.
- `value` is the function value at termination.
- `details` is a `data.frame` with full information about the AO process. For each iteration (column `iteration`) it contains the function value (column `value`), parameter values (columns starting with `p` followed by the parameter index), the active parameter block (columns starting with `b` followed by the parameter index, where 1 stands for a parameter contained in the active parameter block and 0 if not), and computation times in seconds (column `seconds`). Only available if `add_details = TRUE`.
- `seconds` is the overall computation time in seconds.
- `stopping_reason` is a message why the AO process has terminated.

Methods

Public methods:

- [Process\\$new\(\)](#)
- [Process\\$print_status\(\)](#)

- `Process$initialize_details()`
- `Process$update_details()`
- `Process$get_partition()`
- `Process$get_details()`
- `Process$get_value()`
- `Process$get_value_latest()`
- `Process$get_value_best()`
- `Process$get_parameter()`
- `Process$get_parameter_latest()`
- `Process$get_parameter_best()`
- `Process$get_seconds()`
- `Process$get_seconds_total()`
- `Process$check_stopping()`

Method `new()`: Creates a new object of this [R6](#) class.

Usage:

```
Process$new(
  npar = integer(),
  partition = "sequential",
  new_block_probability = 0.3,
  minimum_block_number = 1,
  verbose = FALSE,
  minimize = TRUE,
  iteration_limit = Inf,
  seconds_limit = Inf,
  tolerance_value = 1e-06,
  tolerance_parameter = 1e-06,
  tolerance_parameter_norm = function(x, y) sqrt(sum((x - y)^2)),
  tolerance_history = 1,
  add_details = TRUE
)
```

Arguments:

`npar` [integer(1)]

The (total) length of the target argument(s).

`partition` [character(1) | list()]

Defines the parameter partition, and can be either

- "sequential" for treating each parameter separately,
- "random" for a random partition in each iteration,
- "none" for no partition (which is equivalent to joint optimization),
- or a list of vectors of parameter indices, specifying a custom partition for the AO process.

`new_block_probability` [numeric(1)]

Only relevant if `partition = "random"`.

The probability for a new parameter block when creating a random partition.

Values close to 0 result in larger parameter blocks, values close to 1 result in smaller parameter blocks.

`minimum_block_number` [integer(1)]
 Only relevant if `partition = "random"`.
 The minimum number of blocks in random partitions.

`verbose` [logical(1)]
 Print tracing details during the AO process?

`minimize` [logical(1)]
 Minimize during the AO process?
 If FALSE, maximization is performed.

`iteration_limit` [integer(1) | Inf]
 The maximum number of iterations through the parameter partition before the AO process is terminated.
 Can also be Inf for no iteration limit.

`seconds_limit` [numeric(1)]
 The time limit in seconds before the AO process is terminated.
 Can also be Inf for no time limit.
 Note that this stopping criteria is only checked *after* a sub-problem is solved and not *within* solving a sub-problem, so the actual process time can exceed this limit.

`tolerance_value` [numeric(1)]
 A non-negative tolerance value. The AO process terminates if the absolute difference between the current function value and the one before `tolerance_history` iterations is smaller than `tolerance_value`.
 Can be 0 for no value threshold.

`tolerance_parameter` [numeric(1)]
 A non-negative tolerance value. The AO process terminates if the distance between the current estimate and the before `tolerance_history` iterations is smaller than `tolerance_parameter`.
 Can be 0 for no parameter threshold.
 By default, the distance is measured using the euclidean norm, but another norm can be specified via the `tolerance_parameter_norm` field.

`tolerance_parameter_norm` [function]
 The norm that measures the distance between the current estimate and the one from the last iteration. If the distance is smaller than `tolerance_parameter`, the AO process is terminated.
 It must be of the form `function(x, y)` for two vector inputs `x` and `y`, and return a single numeric value. By default, the euclidean norm `function(x, y) sqrt(sum((x - y)^2))` is used.

`tolerance_history` [integer(1)]
 The number of iterations to look back to determine whether `tolerance_value` or `tolerance_parameter` has been reached.

`add_details` [logical(1)]
 Add details about the AO process to the output?

Method `print_status()`: Prints a status message.

Usage:

```
Process$print_status(message, message_type = 8, verbose = self$verbose)
```

Arguments:

`message` [character(1)]

A status message.

```
message_type [integer(1)]
    The message type, one of the following:
    • 1 for cli::cli_h1()
    • 2 for cli::cli_h2()
    • 3 for cli::cli_h3()
    • 4 for cli::cli_alert_success()
    • 5 for cli::cli_alert_info()
    • 6 for cli::cli_alert_warning()
    • 7 for cli::cli_alert_danger()
    • 8 for cli::cat_line()
verbose [logical(1)]
    Print tracing details during the AO process?
```

Method initialize_details(): Initializes the details part of the output.

Usage:

```
Process$initialize_details(initial_parameter, initial_value)
```

Arguments:

```
initial_parameter [numeric()]
    The starting parameter values for the AO process.
initial_value [numeric(1)]
    The function value at the initial parameters.
```

Method update_details(): Updates the details part of the output.

Usage:

```
Process$update_details(
  value,
  parameter_block,
  seconds,
  error,
  error_message,
  block = self$block
)
```

Arguments:

```
value [numeric(1)]
    The updated function value.
parameter_block [numeric()]
    The updated parameter values for the active parameter block.
seconds [numeric(1)]
    The time in seconds for solving the sub-problem.
error [logical(1)]
    Did solving the sub-problem result in an error?
error_message [character(1)]
    An error message if error = TRUE.
block [integer()]
    The currently active parameter block, represented as parameter indices.
```

Method `get_partition()`: Get a parameter partition.

Usage:

```
Process$get_partition()
```

Method `get_details()`: Get the details part of the output.

Usage:

```
Process$get_details(
  which_iteration = NULL,
  which_block = NULL,
  which_column = c("iteration", "value", "parameter", "block", "seconds")
)
```

Arguments:

`which_iteration` [integer()]

Selects the iteration(s).

Can also be NULL to select all iterations.

`which_block` [character(1) | integer()]

Selects the parameter block in the partition and can be one of

- "first" for the first parameter block,
- "last" for the last parameter block,
- an integer vector of parameter indices,
- or NULL for all parameter blocks.

`which_column` [character()]

Selects the columns in the details part of the output and can be one or more of

- "iteration",
- "value",
- "parameter",
- "block",
- and "seconds".

Method `get_value()`: Get the function value in different steps of the AO process.

Usage:

```
Process$get_value(
  which_iteration = NULL,
  which_block = NULL,
  keep_iteration_column = FALSE,
  keep_block_columns = FALSE
)
```

Arguments:

`which_iteration` [integer()]

Selects the iteration(s).

Can also be NULL to select all iterations.

`which_block` [character(1) | integer()]

Selects the parameter block in the partition and can be one of

- "first" for the first parameter block,

- "last" for the last parameter block,
- an integer vector of parameter indices,
- or NULL for all parameter blocks.

keep_iteration_column [logical(1)]

Keep the column containing the information about the iteration in the output?

keep_block_columns [logical(1)]

Keep the column containing the information about the active parameter block in the output?

Method get_value_latest(): Get the function value in the latest step of the AO process.

Usage:

```
Process$get_value_latest()
```

Method get_value_best(): Get the optimum function value in the AO process.

Usage:

```
Process$get_value_best()
```

Method get_parameter(): Get the parameter values in different steps of the AO process.

Usage:

```
Process$get_parameter(
  which_iteration = self$iteration,
  which_block = NULL,
  keep_iteration_column = FALSE,
  keep_block_columns = FALSE
)
```

Arguments:

which_iteration [integer()]

Selects the iteration(s).

Can also be NULL to select all iterations.

which_block [character(1) | integer()]

Selects the parameter block in the partition and can be one of

- "first" for the first parameter block,
- "last" for the last parameter block,
- an integer vector of parameter indices,
- or NULL for all parameter blocks.

keep_iteration_column [logical(1)]

Keep the column containing the information about the iteration in the output?

keep_block_columns [logical(1)]

Keep the column containing the information about the active parameter block in the output?

Method get_parameter_latest(): Get the parameter value in the latest step of the AO process.

Usage:

```
Process$get_parameter_latest(parameter_type = "full")
```

Arguments:

parameter_type [character(1)]

Selects the parameter type and can be one of

- "full" (default) to get the full parameter vector,
- "block" to get the parameter values for the current block, i.e., the parameters with the indices `self$block`
- "fixed" to get the parameter values which are currently fixed, i.e., all except for those with the indices `self$block`

Method `get_parameter_best()`: Get the optimum parameter value in the AO process.

Usage:

```
Process$get_parameter_best(parameter_type = "full")
```

Arguments:

`parameter_type` [character(1)]

Selects the parameter type and can be one of

- "full" (default) to get the full parameter vector,
- "block" to get the parameter values for the current block, i.e., the parameters with the indices `self$block`
- "fixed" to get the parameter values which are currently fixed, i.e., all except for those with the indices `self$block`

Method `get_seconds()`: Get the optimization time in seconds in different steps of the AO process.

Usage:

```
Process$get_seconds(
  which_iteration = NULL,
  which_block = NULL,
  keep_iteration_column = FALSE,
  keep_block_columns = FALSE
)
```

Arguments:

`which_iteration` [integer()]

Selects the iteration(s).

Can also be NULL to select all iterations.

`which_block` [character(1) | integer()]

Selects the parameter block in the partition and can be one of

- "first" for the first parameter block,
- "last" for the last parameter block,
- an integer vector of parameter indices,
- or NULL for all parameter blocks.

`keep_iteration_column` [logical(1)]

Keep the column containing the information about the iteration in the output?

`keep_block_columns` [logical(1)]

Keep the column containing the information about the active parameter block in the output?

Method `get_seconds_total()`: Get the total optimization time in seconds of the AO process.

Usage:

```
Process$get_seconds_total()
```

Method `check_stopping()`: Checks if the AO process can be terminated.

Usage:

`Process$check_stopping()`

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