

Package ‘ino’

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Title Initialization of Numerical Optimization

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Description Analysis of the initialization for numerical optimization of real-valued functions, particularly likelihood functions of statistical models. See <<https://loelschlaeger.de/ino/>> for more details.

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<https://github.com/loelschlaeger/ino>

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Contents

autoplot.Nop	2
Nop	3
Index	13

autoplot.Nop	<i>Plotting methods</i>
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Description

- autoplot.Nop() plots the objective function
- autoplot.Nop_results() plots boxplots of optimization results
- autoplot.Nop_optima() plots a bar chart of the found optima
- autoplot.Nop_deviation() plots deviations per dimension from a reference

Usage

```
## S3 method for class 'Nop'
autoplot(object, xlim = NULL, xlim2 = NULL, ...)

## S3 method for class 'Nop_optima'
autoplot(object, ...)

## S3 method for class 'Nop_deviation'
autoplot(object, jitter = TRUE, ...)

## S3 method for class 'Nop_results'
autoplot(
  object,
  which_element = "seconds",
  group_by = NULL,
  relative = FALSE,
  ...
)
```

Arguments

object	Depends on the method: • for autoplot.Nop(), a Nop object • for autoplot.Nop_results(), the value Nop\$results • for autoplot.Nop_optima(), the value Nop\$optima • for autoplot.Nop_deviation(), the value Nop\$deviation
xlim, xlim2	[numeric(2)] Ranges for the first and second parameter to plot. If NULL, they are derived from the specified initial values in object.

...	Other arguments passed to specific methods.
jitter	[logical(1)] Apply jitter to the points?
which_element	[character(1)]\cr A column name of 'object' to plot.
group_by	['character(1)] Selects how the plot is grouped. Either: • NULL to not group, • "optimization" to group by optimization label, • "optimizer"" to group by optimizer label.
relative	[logical(1)] Plot values relative to the overall median?

Value

A ggplot object.

Nop

Nop Object

Description

A Nop object defines a numerical optimization problem.

Getting started**Step 1: Create a Nop object:**

Call `object <- Nop$new(f, target, npar, ...)` where

- `f` is the objective function,
- `target` are the names of the target arguments,
- `npair` specifies the lengths of the target arguments,
- and `...` are additional arguments for `f`.

You can now evaluate the objective function via the `$evaluate()` method.

Step 2: Specify numerical optimizers:

Call `object$set_optimizer(<optimizer object>)`, where `<optimizer object>` is an object of class `optimizer`, which can be created via the `{optimizerR}` package (please refer to [the package homepage](#) for details).

For example,

- `optimizerR::Optimizer$new(which = "stats::nlm")` defines the `nlm` optimizer,
- `optimizerR::Optimizer$new(which = "stats::optim")` defines the `optim` optimizer.

Step 3: Select initial values:

Call initialization methods to define starting values for the optimization (the different initialization strategies are illustrated in the package vignettes), for example:

- `object$initialize_fixed()` for fixed initial values,
- `object$initialize_random()` for random initial values,
- `object$initialize_continue()` for initial values based on parameter estimates from previous optimization runs.

Step 4: Optimization:

Call `object$optimize()` for the optimization.

Step 5: Analyze the results:

- `$results` returns a tibble of the optimization results,
- `$optima()` lists all identified optima,
- `$minimum` and `$maximum` return the best minimizer and maximizer

Progress during optimization

Displaying progress during multiple optimization runs via the `{progressr}` package is supported. To get started, run

```
progressr::handlers(global = TRUE)
```

and see [handlers](#) for details.

Parallel optimization

Parallel computation of multiple optimization runs via the `{future}` package is supported. To get started, run one of

```
future::plan(future::multisession)
```

and see [plan](#) for details.

Active bindings

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

The currently defined initial values.

Use the `initialize_*`() methods to add, transform, and reset values.

`results` [tibble, read-only]

Optimization results with identifiers:

- `".optimization_label"` (identifies the optimization run)
- `".optimizer_label"` (identifies the optimizer)
- `".direction"` (identifies the optimization direction)
- `".original"` (identifies results obtained on the original problem)

The output has an associated [autoplot](#) method.

`minimum` [list(2), read-only]

Best value and parameter across all (original) minimizations.

`maximum` [list(2), read-only]

Best value and parameter across all (original) maximizations.

`npar` [integer(), read-only]
 The length of each target argument.

`verbose` [logical(1)]
 Print progress and details?

`fresh_label` [character(1), read-only]
 An optimization label that has not been used yet.

Methods

Public methods:

- `Nop$new()`
- `Nop$fixed_argument()`
- `Nop$reduce_argument()`
- `Nop$standardize_argument()`
- `Nop$print()`
- `Nop$evaluate()`
- `Nop$set_optimizer()`
- `Nop$initialize_fixed()`
- `Nop$initialize_random()`
- `Nop$initialize_grid()`
- `Nop$initialize_custom()`
- `Nop$initialize_continue()`
- `Nop$initialize_filter()`
- `Nop$initialize_promising()`
- `Nop$initialize_transform()`
- `Nop$initialize_reset()`
- `Nop$optimize()`
- `Nop$optima()`
- `Nop$deviation()`
- `Nop$clone()`

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

The output has an associated `autoplot` method.

Usage:

`Nop$new(f, target = NULL, npar, gradient = NULL, hessian = NULL, ...)`

Arguments:

`f` [function]

A function to be optimized (the so-called objective function).

It is expected that

1. `f` has at least one numeric argument,
2. the return value of `f` is of the structure `numeric(1)`.

`target` [character()]

The argument name(s) that get optimized (the so-called target arguments).

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 argument(s) specified via target.

`gradient` [function|NULL]
 Optionally a function that returns the gradient of f.
 The function call of gradient must be identical to f.
 Ignored for optimizers that do not support user-supplied gradient.

`hessian` [function|NULL]
 Optionally a function that returns the Hessian of f.
 The function call of hessian must be identical to f.
 Ignored for optimizers that do not support user-supplied Hessian.

... Optionally additional function arguments passed to f (and gradient and hessian, if specified) that are fixed during the optimization.

Method `fixed_argument()`: Manages fixed arguments for the objective function.

Usage:

`Nop$fixed_argument(action, ...)`

Arguments:

`action` [character(1)]

One of:

- "set" to set an argument,
- "get" to extract an argument value,
- "remove" to remove an argument,
- "reset" to reset an argument to its original value,
- "modify" to modify an argument value.

Note that "set" overrides an argument value, while "modify" preserves the original value, which can be recovered via "reset".

... Additional parameters depending on action:

- named arguments if action = "set" or "modify",
- a single argument name if action = "get", "remove", or "reset".

Method `reduce_argument()`: Reduces a fixed argument for the objective function.

Usage:

```
Nop$reduce_argument(
  argument_name,
  proportion = 0.5,
  how = "random",
  centers = 2L,
  byrow = TRUE,
  ignore = integer()
)
```

Arguments:

`argument_name` [character(1)]

The name of a fixed argument for the objective function.

`proportion`, `how`, `centers`, `byrow`, `ignore` Passed on to [portion](#).

Method `standardize_argument()`: Standardizes a fixed argument for the objective function.

Usage:

```
Nop$standardize_argument(
  argument_name,
  center = TRUE,
  scale = TRUE,
  byrow = FALSE,
  ignore = integer(),
  jointly = list()
)
```

Arguments:

`argument_name` [character(1)]

The name of a fixed argument for the objective function.

`center`, `scale`, `byrow`, `ignore`, `jointly` Passed on to [normalize](#).

Method `print()`: Prints details of the Nop object.

Usage:

```
Nop$print(...)
```

Arguments:

... Currently not used.

Method `evaluate()`: Evaluates the objective function.

Usage:

```
Nop$evaluate(
  at = rep(0, sum(self$npar)),
  .gradient_as_attribute = FALSE,
  .hessian_as_attribute = FALSE
)
```

Arguments:

`at` [numeric()]

The values for the target argument(s), written in a single vector.

Must be of length `sum(self$npar)`.

`.gradient_as_attribute`, `.hessian_as_attribute` [logical(1)]

Add gradient and / or Hessian value as attributes?

If gradient and / or Hessian function is not specified, numerical approximation is used.

Method `set_optimizer()`: Specifies a numerical optimizer.

Usage:

```
Nop$set_optimizer(optimizer, optimizer_label = optimizer$label)
```

Arguments:

`optimizer` [Optimizer]

An Optimizer object, which can be created via [Optimizer](#).

`optimizer_label` [character(1)]

A (unique) label for the optimizer.

Method `initialize_fixed()`: Defines fixed initial values for the optimization.

Usage:

```
Nop$initialize_fixed(at)
```

Arguments:

```
at [integer(self$sum(npar)) | list()]
```

The fixed initial parameter vector.

It can also be a list of such vectors.

Method `initialize_random()`: Defines random initial values for the optimization.

Usage:

```
Nop$initialize_random(
  runs = 1L,
  sampler = function() stats::rnorm(sum(self$npar))
)
```

Arguments:

```
runs [integer(1)]
```

The number of optimization runs.

```
sampler [function]
```

A function without any arguments that returns a numeric vector of length `sum(self$npar)`.

Method `initialize_grid()`: Defines a grid of initial values for the optimization.

Usage:

```
Nop$initialize_grid(lower = 0, upper = 1, breaks = 3, jitter = FALSE, ...)
```

Arguments:

```
lower, upper [numeric(1) | numeric(self$sum(npar))]
```

Lower and upper grid bounds for each parameter dimension.

```
breaks [integer(1) | integer(self$sum(npar))]
```

The number of breaks for each parameter dimension.

`jitter` Add noise to the grid points for a random grid layout?

... Optional parameters passed to [jitter](#).

Method `initialize_custom()`: Defines custom initial values for the optimization.

Usage:

```
Nop$initialize_custom(at, seconds = rep(0, length(at)), type = "custom")
```

Arguments:

```
at [list()]
```

A list of initial parameter vectors.

```
seconds [numeric(length(at))]
```

The number of seconds it took to obtain each initial value in `at`, which is added to the overall optimization time.

```
type [character(1)]
```

The type of the initial values.

Method `initialize_continue()`: Defines initial values based on results from previous optimizations.

Usage:

Nop\$initialize_continue(optimization_label)

Arguments:

optimization_label [character(1)]

Label of optimization runs from which to select.

Method initialize_filter(): Filters initial values from the defined initial values.

Usage:

Nop\$initialize_filter(condition)

Arguments:

condition [character(1)]

Defines the condition on which the initial values are filtered, one of:

- "gradient_negative" for points where the gradient is negative,
- "gradient_positive" for points where the gradient is negative,
- "hessian_negative" for points where the Hessian is negative definite,
- "hessian_positive" for points where the Hessian is positive definite.

Method initialize_promising(): Selects promising initial values from the defined initial values.

Usage:

Nop\$initialize_promising(proportion, condition)

Arguments:

proportion [numeric(1)]

The proportion of selected from the defined initial values.

condition [character(1)]

Defines the condition on which the initial values are selected, one of:

- "value_small" for points where the function value is smallest,
- "value_large" for points where the function value is largest,
- "gradient_small" for points where the gradient norm is smallest,
- "gradient_large" for points where the gradient norm is largest,
- "condition_small" for points where the Hessian condition is smallest,
- "condition_large" for points where the Hessian condition is largest.

Method initialize_transform(): Transforms the currently defined initial values.

Usage:

Nop\$initialize_transform(transformer = function(x) x)

Arguments:

transformer [function()]

A function that receives and returns a numeric() of length sum(self\$npar).

Method initialize_reset(): Resets the currently defined initial values.

Usage:

Nop\$initialize_reset()

Method `optimize()`: Optimizes the target function.

Usage:

```
Nop$optimize(
  optimization_label = self$fresh_label,
  which_optimizer = "all",
  which_direction = "min",
  lower = NULL,
  upper = NULL,
  seconds = Inf,
  hide_warnings = TRUE,
  reset_initial_afterwards = TRUE
)
```

Arguments:

`optimization_label` [character(1)]

A label for the optimization to distinguish optimization runs.

Setting a label is useful when using the `$initialize_continue()` method.

`which_optimizer` [character() | integer()]

Selects numerical optimizers. Either:

- "all" for all specified optimizers,
- specific optimizer labels,
- specified optimizer ids as defined in the `print()` output.

`which_direction` [character()]

Selects the direction of optimization. One or both of:

- "min" for minimization,
- "max" for maximization.

`lower, upper` [numeric() | NULL]

Optionally lower and upper parameter bounds.

Ignored for optimizers that do not support parameter bounds.

`seconds` [numeric(1)]

A time limit in seconds.

Optimization is interrupted prematurely if seconds is exceeded.

Note the limitations documented in [setTimeLimit](#).

`hide_warnings` [logical(1)]

Hide any warnings during optimization?

`reset_initial_afterwards` [logical(1)]

Reset the initial values after the optimization?

Details: Supports:

- Parallel computation of multiple optimization runs via `{future}`
- Progress messages via `{progressr}`

Method `optima()`: Lists all identified optima.

The output has an associated [autoplot](#) method.

Usage:

```
Nop$optima(
  which_direction = "min",
  only_original = TRUE,
  group_by = NULL,
  sort_by_value = FALSE,
  digits = getOption("digits", default = 7)
)
```

Arguments:

`which_direction` [character()]

Selects the direction of optimization. One or both of:

- "min" for minimization,
- "max" for maximization.

`only_original` [‘logical(1)']

Include only optima obtained on the original problem?

`group_by` [‘character(1)']

Selects how the output is grouped. Either:

- NULL to not group,
- "optimization" to group by optimization label,
- "optimizer" to group by optimizer label.

`sort_by_value` [‘logical(1)']

Sort by value? Else, sort by frequency.

`digits` [‘integer(1)']

The number of decimal places.

Method `deviation()`: Compute deviations with respect to a reference parameter.

The output has an associated [autoplot](#) method.

Usage:

```
Nop$deviation(
  reference = rep(0, sum(self$npar)),
  which_element = "initial",
  which_direction = "min",
  which_optimizer = "all",
  only_original = TRUE,
  parameter_labels = paste0("x", seq_len(sum(self$npar)))
)
```

Arguments:

`reference` [numeric()]

The reference vector of length `sum(self$npar)`.

`which_element` [‘character(1)']

Either

- "initial" for deviations with respect to the initial values, or
- "parameter" for deviations with respect to the estimated parameters.

`which_direction` [character()]

Selects the direction of optimization. One or both of:

- "min" for minimization,

- "max" for maximization.

which_optimizer [character() | integer()]
 Selects numerical optimizers. Either:

- "all" for all specified optimizers,
- specific optimizer labels,
- specified optimizer ids as defined in the print() output.

only_original [logical(1)]
 Include only optima obtained on the original problem?

parameter_labels [character()]
 Labels for the parameters of length sum(self\$npar).

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

Usage:

Nop\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

Examples

```
### define objective function, optimizer and initial values
Nop_ackley <- Nop$new(f = TestFunctions::TF_ackley, npar = 2)$
  set_optimizer(optimizerR::Optimizer$new(which = "stats::nlm"))$
  initialize_random(runs = 20)

### plot function surface and initial values
Nop_ackley |> ggplot2::autoplot()

### minimize objective function
Nop_ackley$optimize(which_direction = "min")

### show optima
Nop_ackley$optima(digits = 0)

### show best value and parameter across all minimizations
Nop_ackley$minimum
```

Index

autoplot, [4](#), [5](#), [10](#), [11](#)
autoplot.Nop, [2](#)
autoplot.Nop_deviation (autoplot.Nop), [2](#)
autoplot.Nop_optima (autoplot.Nop), [2](#)
autoplot.Nop_results (autoplot.Nop), [2](#)

handlers, [4](#)

jitter, [8](#)

nlm, [3](#)
Nop, [3](#)
normalize, [7](#)

optim, [3](#)
Optimizer, [7](#)

plan, [4](#)
portion, [6](#)

setTimeLimit, [10](#)