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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`autoplot.Nop` *Plotting methods*

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,
- npar 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 {optimizeR} package (please refer to the package homepage for details).

For example,

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

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