Package 'optimizeR'

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Description

This function performs numerical optimization using an optimizer object.

Usage

```
apply_optimizer(optimizer = optimizer_nlm(), objective, initial, ...)
```

Arguments

optimizer	An object of class optimizer.
objective	A function to be optimized, returning a single numeric. Its first argument must be a numeric vector of the same length as initial, followed by any other arguments specified by the argument.
initial	A numeric vector with starting parameter values for the optimization.
	Additional arguments to be passed to optimizer.

Value

A named list, containing at least these four elements:

value $\,A\,$ numeric, the value of the estimated optimum of objective.

parameter A numeric vector, the parameter vector where the optimum of objective is obtained. seconds A numeric, the total optimization time in seconds.

initial A numeric, the initial parameter values.

Appended are additional output elements of the optimizer (if not excluded by the output_ignore element via define_optimizer).

See Also

define_optimizer() for creating an optimizer object.

Examples

```
apply_optimizer(optimizer_nlm(), function(x) x^4 + 3*x - 5, 2)
```

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define_optimizer

Specify numerical optimizer

Description

This function specifies the framework for a numerical optimizer.

Two wrappers for well-known optimizers are already available:

- 1. optimizer_nlm() for the nlm optimizer
- 2. optimizer_optim() for the optim optimizer

Usage

```
define_optimizer(
  .optimizer,
  .objective,
  .initial,
  .value,
  .parameter,
  .direction,
  .output_ignore = character(0),
  .validate = FALSE,
 .validation_settings = list(objective_test = TestFunctions::TF_ackley, objective_add =
    list(), initial = round(stats::rnorm(2), 2), check_seconds = 10)
)
optimizer_nlm(
  .output_ignore = character(0),
  .validate = FALSE,
  .validation_settings = list()
)
optimizer_optim(
  .direction = "min",
  .output_ignore = character(0),
  .validate = FALSE,
  .validation_settings = list()
)
```

Arguments

.optimizer

A function, a numerical optimizer. Four conditions must be met:

1. It must have an input named .objective for a function, the objective function which is optimized over its first argument.

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- 2. It must have an input named .initial for a numerical vector, the initial parameter vector.
- 3. It must have a . . . argument for additional parameters to the objective function.
- 4. The output must be a named list, including the optimal function value and the optimal parameter vector.

. objective A character, the name of the function input of optimizer.

.initial A character, the name of the starting parameter values input of optimizer.

.value A character, the name of the optimal function value in the output list of optimizer.

. parameter A character, the name of the optimal parameter vector in the output list of optimizer.

. direction A character, indicates whether the optimizer minimizes ("min") or maximizes ("max").

Additional arguments to be passed to the optimizer. Without specifications, the default values of the optimizer are used.

.output_ignore A character vector of element names in the output of .optimizer that are not saved. The elements .value and .parameter are added automatically to .output_ignore, because they are saved separately, see the output documentation of apply_optimizer.

.validate A logical, set to TRUE (FALSE) to (not) validate the optimizer object. By default, .validate = FALSE.

.validation_settings

Ignored if .valdiate = FALSE. Otherwise, a list of validation settings:

objective_test A function, the test function to be optimized. By default, it is the Ackley function.

objective_add A list of additional arguments to objective_test (if any).
By default, objective_add = list(), because the default function for objective_test
does not have additional arguments.

initial A numeric vector, the initial values for the optimization of objective_test.
By default, initial = round(stats::rnorm(2), 2).

check_seconds An integer, the maximum number of seconds before the test is aborted. The test call is considered to be successful if no error occurred within check_seconds seconds. By default, check_seconds = 10.

Value

An optimizer object.

Format

An optimizer object is a list of six elements:

optimizer A function, the optimization algorithm.

optimizer_name A character, the name of optimizer.

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optimizer_arguments A named list, where each element is an additional function argument for optimizer.

optimizer_direction Either "min" if the optimizer minimizes or "max" if the optimizer maximizes. **optimizer_labels** A named list of four character:

objective the name of the function input of optimizerinitial the name of the starting parameter values input of optimizervalue the name of the optimal function value in the output list of optimizerparameter the name of the optimal parameter vector in the output list of optimizer.

output_ignore A character vector of element names in the output list of optimizer that are ignored. The elements value and parameter are added automatically to output_ignore, because they are saved separately, see the output documentation of apply_optimizer.

See Also

Use apply_optimizer() to apply an optimizer object for numerical optimization.

Examples

```
define_optimizer(
  .optimizer = pracma::nelder_mead,
                                              # optimization function
  .objective = "fn",
                                              # name of function input
  .initial = "x0",
                                              # name of initial input
  .value = "fmin",
                                              # name of value output
  .parameter = "xmin",
                                              # name of parameter output
  .direction = "min",
                                              # optimizer minimizes
  .output_ignore = c("restarts", "errmess"), # ignore some outputs
 tol = 1e-6,
                                              # additional optimizer argument
  .validate = TRUE
                                              # validate the object
)
```

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Specify objective function

Description

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

Value

An Objective object.

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Active bindings

objective_name A character, a label for the objective function.

fixed_arguments A character, the names of the fixed arguments (if any).

seconds A numeric, 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 Either TRUE to hide warnings when evaluating the objective function, or FALSE (default) if not.

verbose Either TRUE (default) to print status messages, or FALSE to hide those.

npar An integer vector, defining the length of each target argument.

output_template A template of the expected output value, used for the validate method.

Methods

Public methods:

- Objective\$new()
- Objective\$set_argument()
- Objective\$get_argument()
- Objective\$remove_argument()
- Objective\$validate()
- Objective\$evaluate()
- Objective\$print()
- Objective\$clone()

Method new(): Creates a new Objective object.

```
Usage:
```

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

Arguments:

f 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 (although this can be altered via the output_template field).

target A character, the argument name(s) of f that get optimized.

All target arguments must receive a numeric vector.

Can be NULL (default), then it is the first argument of f.

npar A integer of the same length as target, defining the length of the respective numeric vector argument.

... Optionally additional arguments to f that are fixed during the optimization.

Returns: A new Objective object.

Method set_argument(): Set a fixed function argument.

Usage:

Objective\$set_argument(..., overwrite = TRUE, verbose = self\$verbose) Arguments: ... Optionally additional arguments to f that are fixed during the optimization. overwrite Either TRUE (default) to allow overwriting, or FALSE if not. verbose Either TRUE (default) to print status messages, or FALSE to hide those. Returns: Invisibly the Objective object. **Method** get_argument(): Get a fixed function argument. Usage: Objective\$get_argument(argument_name, verbose = self\$verbose) Arguments: argument_name A character, a name of an argument for f. verbose Either TRUE (default) to print status messages, or FALSE to hide those. Returns: The argument value. **Method** remove_argument(): Remove a fixed function argument. Usage: Objective\$remove_argument(argument_name, verbose = self\$verbose) Arguments: argument_name A character, a name of an argument for f. verbose Either TRUE (default) to print status messages, or FALSE to hide those. Returns: Invisibly the Objective object. Method validate(): Validate an Objective object. Usage: Objective\$validate(.at) Arguments: .at A numeric of length sum(self\$npar), the values for the target arguments written in a single vector. Returns: Invisibly the Objective object. **Method** evaluate(): Evaluate the objective function. Usage: Objective\$evaluate(.at, .negate = FALSE, ...) Arguments: .at A numeric of length sum(self\$npar), the values for the target arguments written in a single vector. . negate Either TRUE to negate the numeric return value of f, or FALSE (default) else. ... Optionally additional arguments to f that are fixed during the optimization. Returns: The objective value.

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

```
Usage:
Objective$print()
Returns: Invisibly the Objective object.

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
11k <- function(mu, sd, lambda, data) {</pre>
  sd \leftarrow exp(sd)
  lambda <- plogis(lambda)</pre>
  cluster_1 <- lambda * dnorm(data, mu[1], sd[1])</pre>
  cluster_2 <- (1 - lambda) * dnorm(data, mu[2], sd[2])</pre>
  sum(log(cluster_1 + cluster_2))
### the log-likelihood function is supposed to be optimized over the first
### three arguments, the 'data' argument is constant
objective <- Objective$new(</pre>
  f = 11k, target = c("mu", "sd", "lambda"), npar = c(2, 2, 1),
  data = faithful$eruptions
)
### evaluate the objective function 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 as R6 object

Description

A Optimizer R6 object defines a numerical optimizer based on an optimization function 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 A character, the label for the optimizer.

algorithm A function, the optimization algorithm.

arg_objective A character, the argument name for the objective function in algorithm.

arg_initial A character, the argument name for the initial values in algorithm.

out_value A character, the element name for the optimal function value in the output list of algorithm.

out_parameter A character, the element name for the optimal parameters in the output list of algorithm.

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

arguments A named list of custom arguments for algorithm. Defaults are used for arguments that are not specified.

seconds A numeric, 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 Either TRUE to hide warnings during optimization, or FALSE (default) else.

output_ignore A character vector of elements to ignore in the optimization output.

Methods

Public methods:

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

Method new(): Initializes a new Optimizer object.

```
Usage:
```

```
Optimizer$new(which, ...)
```

Arguments:

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

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

Returns: A new Optimizer object.

```
Method definition(): Defines an optimizer.
```

```
Usage:
Optimizer$definition(
   algorithm,
   arg_objective,
   arg_initial,
   out_value,
   out_parameter,
   direction
)
```

Arguments:

algorithm A function, the optimization algorithm.

arg_objective A character, the argument name for the objective function in algorithm.

arg_initial A character, the argument name for the initial values in algorithm.

out_value A character, the element name for the optimal function value in the output list of algorithm.

out_parameter A character, the element name for the optimal parameters in the output list of algorithm.

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

Returns: Invisibly the Optimizer object.

Method set_arguments(): Sets optimizer arguments.

```
Usage:
```

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

Arguments:

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

Returns: The Optimizer object.

Method validate(): Validates the Optimizer object. A time limit in seconds for the optimization can be set via the \$seconds field.

Usage:

```
Optimizer$validate(
  objective = optimizeR::test_objective,
  initial = round(stats::rnorm(2)),
    ...,
  direction = "min"
)
```

Arguments:

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 a Objective object for more flexibility.

initial A numeric vector with starting parameter values for the optimization.

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

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

Returns: The Optimizer object.

Method minimize(): Performing minimization.

```
Usage:
```

```
Optimizer$minimize(objective, initial, ...)
```

Arguments:

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 a Objective object for more flexibility.

initial A numeric vector with starting parameter values for the optimization.

... Optionally additional arguments to be passed to the optimizer algorithm. Without specifications, default values 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 also 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, ...)
```

Arguments:

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 a Objective object for more flexibility.

initial A numeric vector with starting parameter values for the optimization.

... Optionally additional arguments to be passed to the optimizer algorithm. Without specifications, default values 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, direction = "min", ...)
```

Arguments:

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 a Objective object for more flexibility.

initial A numeric vector with starting parameter values for the optimization.

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

... Optionally additional arguments to be passed to the optimizer algorithm. Without specifications, default values 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")</pre>
```

Method print(): Prints the optimizer label.

```
Usage:
       Optimizer$print(...)
       Arguments:
       ... Optionally additional arguments to be passed to the optimizer algorithm. Without specifi-
           cations, default values are used.
       Returns: Invisibly the Optimizer object.
     Method clone(): The objects of this class are cloneable with this method.
       Usage:
       Optimizer$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 \leftarrow c(3, 3)
    # 2. get overview of optimizers in dictionary
    optimizer_dictionary$keys
    # 3. define 'nlm' optimizer
    nlm <- Optimizer$new(which = "stats::nlm")</pre>
    # 4. define the 'pracma::nelder_mead' optimizer (not contained in the dictionary)
    nelder_mead <- Optimizer$new(which = "custom")</pre>
    nelder_mead$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)

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Description

The optimizer_dictionary object is a dictionary of currently implemented numerical optimizer functions.

Usage

```
optimizer_dictionary
```

Format

An R6 object of class Dictionary.

ParameterSpaces

Switch Between Parameter Spaces

Description

This R6 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. Parameters in this space are typically identified.

In the Interpretation Space, parameters are stored as a list and can take different formats (e.g., matrix). Parameters here do not need to be identified.

The user can define transformation functions (not necessarily bijective) to switch between these two spaces via the \$02i() and \$i2o() methods.

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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.
 ParameterSpacesswitch(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
```

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$02i(...)
```

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

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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().

The default is do. 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) {</pre>
 mu <- theta[1:2]</pre>
 sd <- exp(theta[3:4])</pre>
 lambda <- plogis(theta[5])</pre>
 c1 <- lambda * dnorm(data, mu[1], sd[1])</pre>
 c2 <- (1 - lambda) * dnorm(data, mu[2], sd[2])</pre>
 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$</pre>
    parameter_names = c("mu", "sd", "lambda"),
```

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

test_objective

Test objective function

Description

This function is useful for testing or debugging the behavior of objective functions. It can throw a warning and / or an error on purpose.

Usage

```
test_objective(
    x,
    value = x,
    warning_prob = 0,
    error_prob = 0,
    warning_msg = "warning",
    error_msg = "error",
    call. = TRUE
)
```

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Arguments

X	Any input.
value	The return value, any object.
warning_prob	The probability for throwing a warning.
error_prob	The probability for throwing an error.
warning_msg	The warning message.
error_msg	The error message.
call.	Passed to warning or stop, respectively.

Value

The argument value.

est optimization function

Description

This function is useful for testing or debugging the behavior of optimization functions. It can throw a warning and / or an error on purpose.

Usage

```
test_optimizer(
  objective = test_objective,
  initial = 1,
    ...,
  parameter = 1,
  value = objective(parameter),
  seconds = 0,
  warning_prob = 0,
  error_prob = 0,
  warning_msg = "warning",
  error_msg = "error",
  call. = TRUE
)
```

Arguments

```
objective An objective function.

initial The initial parameter vector.

Optionally additional arguments to be passed to objective.

parameter Defines the output parameter.

value Defines the output value.
```

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seconds A delay in number of seconds.

warning_prob The probability for throwing a warning.
error_prob The probability for throwing an error.

warning_msg The warning message.
error_msg The error message.

call. Passed to warning or stop, respectively.

Value

A list with elements parameter and value.

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