Package ‘mize’
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Description Optimization algorithms implemented in R, including conjugate gradient (CG), Broyden-Fletcher-Goldfarb-Shanno (BFGS) and the limited memory BFGS (L-BFGS) methods. Most internal parameters can be set through the call interface. The solvers hold up quite well for higher-dimensional problems.
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check_mize_convergence

Check Optimization Convergence

Description

Updates the optimizer with information about convergence or termination, signaling if the optimization process should stop.

Usage

check_mize_convergence(mize_step_info)

Arguments

mize_step_info  Step info for this iteration, created by mize_step_summary

Details

On returning from this function, the updated value of opt will contain:

- A boolean value is_terminated which is TRUE if termination has been indicated, and FALSE otherwise.
- A list terminate if is_terminated is TRUE. This contains two items: what, a short string describing what caused the termination, and val, the value of the termination criterion that caused termination. This list will not be present if is_terminated is FALSE.

Convergence criteria are only checked here. To set these criteria, use make_mize or mize_init.

Value

opt updated with convergence and termination data. See 'Details'.

Examples

rb_fg <- list(
    fn = function(x) { 100 * (x[2] - x[1] * x[1]) ^ 2 + (1 - x[1]) ^ 2 },
    gr = function(x) { c(-400 * x[1] * (x[2] - x[1] * x[1]) - 2 * (1 - x[1]),
    rb0 <- c(-1.2, 1)
)

opt <- make_mize(method = "BFGS", par = rb0, fg = rb_fg, max_iter = 30)
mize_res <- mize_step(opt = opt, par = rb0, fg = rb_fg)
step_info <- mize_step_summary(mize_res$opt, mize_res$par, rb_fg, rb0)
# check convergence by looking at opt$is_terminated
opt <- check_mize_convergence(step_info)
make_mize

Create an Optimizer

Description
Factory function for creating a (possibly uninitialized) optimizer.

Usage

```r
make_mize(method = "L-BFGS", norm_direction = FALSE,
          scale_hess = TRUE, memory = 5, cg_update = "PR+",
          preconditioner = ", tn_init = 0, tn_exit = "curvature",
          nest_q = 0, nest_convex_approx = FALSE, nest_burn_in = 0,
          step_up = 1.1, step_up_fun = c("*", "+") step_down = NULL,
          dbd_weight = 0.1, line_search = "More-Thuente", c1 = 1e-04,
          c2 = NULL, step@ = NULL, step_next_init = NULL,
          try_newton_step = NULL, ls_max_fn = 20, ls_max_gr = Inf,
          ls_max_fg = Inf, ls_max_alpha_mult = Inf, ls_max_alpha = Inf,
          ls_safe_cubic = FALSE, strong_curvature = NULL,
          approx_armijo = NULL, mom_type = NULL, mom_schedule = NULL,
          mom_init = NULL, mom_final = NULL, mom_switch_iter = NULL,
          mom_linear_weight = FALSE, use_init_mom = FALSE, restart = NULL,
          restart_wait = 10, par = NULL, fg = NULL, max_iter = 100,
          max_fn = Inf, max_gr = Inf, max_fg = Inf, abs_tol = NULL,
          rel_tol = abs_tol, grad_tol = NULL, ginf_tol = NULL,
          step_tol = NULL)
```

Arguments

- **method**
  Optimization method. See 'Details' of `mize`.

- **norm_direction**
  If TRUE, then the steepest descent direction is normalized to unit length. Useful
  for adaptive step size methods where the previous step size is used to initialize
  the next iteration.

- **scale_hess**
  if TRUE, the approximation to the inverse Hessian is scaled according to the
  method described by Nocedal and Wright (approximating an eigenvalue). Ap-
  plies only to the methods BFGS (where the scaling is applied only during the first
  step) and L-BFGS (where the scaling is applied during every iteration). Ignored
  otherwise.

- **memory**
  The number of updates to store if using the L-BFGS method. Ignored otherwise.
  Must be a positive integer.

- **cg_update**
  Type of update to use for the "CG" method. For details see the "CG" subsection
  of the "Optimization Methods" section. Ignored if method is not "CG".

- **preconditioner**
  Type of preconditioner to use in Truncated Newton. Leave blank or set to
  "L-BFGS" to use a limited memory BFGS preconditioner. Use the "memory" pa-
  rameter to control the number of updates to store. Applies only if method = "TN",
  or "CG", ignored otherwise.
Type of initialization to use in inner loop of Truncated Newton. Use 0 to use the zero vector (the usual TN initialization), or "previous" to use the final result from the previous iteration, as suggested by Martens (2010). Applies only if method = "TN", ignored otherwise.

Type of exit criterion to use when terminating the inner CG loop of Truncated Newton method. Either "curvature" to use the standard negative curvature test, or "strong" to use the modified "strong" curvature test in TNPACK (Xie and Schlick, 1999). Applies only if method = "TN", ignored otherwise.

Strong convexity parameter for the "NAG" method's momentum term. Must take a value between 0 (strongly convex) and 1 (results in steepest descent). Ignored unless the method is "NAG" and nest_convex_approx is FALSE.

If TRUE, then use an approximation due to Sutskever for calculating the momentum parameter in the NAG method. Only applies if method is "NAG".

Number of iterations to wait before using a non-zero momentum. Only applies if using the "NAG" method or setting the momentum_type to "Nesterov".

Value by which to increase the step size for the "bold" step size method or the "DBD" method.

Operator to use when combining the current step size with step_up. Can be one of "*" (to multiply the current step size with step_up) or "+" (to add).

Multiplier to reduce the step size by if using the "DBD" method or the "bold". Can also be used with the "back" line search method, but is optional. Should be a positive value less than 1.

Weighting parameter used by the "DBD" method only, and only if no momentum scheme is provided. Must be an integer between 0 and 1.

Type of line search to use. See 'Details' of mize.

Sufficient decrease parameter for Wolfe-type line searches. Should be a value between 0 and 1.

Sufficient curvature parameter for line search for Wolfe-type line searches. Should be a value between c1 and 1.

Initial value for the line search on the first step. See 'Details' of mize.

For Wolfe-type line searches only, how to initialize the line search on iterations after the first. See 'Details' of mize.

For Wolfe-type line searches only, try the line step value of 1 as the initial step size whenever step_next_init suggests a step size > 1. Defaults to TRUE for quasi-Newton methods such as BFGS and L-BFGS, FALSE otherwise.

Maximum number of function evaluations allowed during a line search.

Maximum number of gradient evaluations allowed during a line search.

Maximum number of function or gradient evaluations allowed during a line search.

The maximum value that can be attained by the ratio of the initial guess for alpha for the current line search, to the final value of alpha of the previous line search. Used to stop line searches diverging due to very large initial guesses. Only applies for Wolfe-type line searches.
ls_max_alpha
Maximum value of alpha allowed during line search. Only applies for line_search = "more-thuente".

ls_safe_cubic
(Optional). If TRUE, check that cubic interpolation in the Wolfe line search does not produce too small a value. Only applies for line_search = "more-thuente".

strong_curvature
(Optional). If TRUE use the strong curvature condition in Wolfe line search. See the 'Line Search' section of mize for details.

approx_armijo
(Optional). If TRUE use the approximate Armijo condition in Wolfe line search. See the 'Line Search' section of mize for details.

mom_type
Momentum type, either "classical" or "nesterov".

mom_schedule
Momentum schedule. See 'Details' of mize.

mom_init
Initial momentum value.

mom_final
Final momentum value.

mom_switch_iter
For mom_schedule "switch" only, the iteration when mom_init is changed to mom_final.

mom_linear_weight
If TRUE, the gradient contribution to the update is weighted using momentum contribution.

use_init_mom
If TRUE, then the momentum coefficient on the first iteration is non-zero. Otherwise, it's zero. Only applies if using a momentum schedule.

restart
Momentum restart type. Can be one of "fn" or "gr". See 'Details' of mize.

restart_wait
Number of iterations to wait between restarts. Ignored if restart is NULL.

par
(Optional) Initial values for the function to be optimized over.

fg
(Optional). Function and gradient list. See 'Details' of mize.

max_iter
(Optional). Maximum number of iterations. See the 'Convergence' section of mize for details.

max_fn
(Optional). Maximum number of function evaluations. See the 'Convergence' section of mize for details.

max_gr
(Optional). Maximum number of gradient evaluations. See the 'Convergence' section of mize for details.

max_fg
(Optional). Maximum number of function or gradient evaluations. See the 'Convergence' section of mize for details.

abs_tol
(Optional). Absolute tolerance for comparing two function evaluations. See the 'Convergence' section of mize for details.

rel_tol
(Optional). Relative tolerance for comparing two function evaluations. See the 'Convergence' section of mize for details.

grad_tol
(Optional). Absolute tolerance for the length (l2-norm) of the gradient vector. See the 'Convergence' section of mize for details.

ginf_tol
(Optional). Absolute tolerance for the infinity norm (maximum absolute component) of the gradient vector. See the 'Convergence' section of mize for details.

step_tol
(Optional). Absolute tolerance for the size of the parameter update. See the 'Convergence' section of mize for details.
Details

If the function to be optimized and starting point are not present at creation time, then the optimizer should be initialized using `mize_init` before being used with `mize_step`.

See the documentation to `mize` for an explanation of all the parameters.

Details of the `fg` list containing the function to be optimized and its gradient can be found in the 'Details' section of `mize`. It is optional for this function, but if it is passed to this function, along with the vector of initial values, `par`, the optimizer will be returned already initialized for this function. Otherwise, `mize_init` must be called before optimization begins.

Additionally, optional convergence parameters may also be passed here, for use with `check_mize_convergence`. They are optional here if you plan to call `mize_init` later, or if you want to do your own convergence checking.

Examples

```r
# Function to optimize and starting point
rosenbrock_fg <- list(
  fn = function(x) { 100 * (x[2] - x[1] * x[1]) ^ 2 + (1 - x[1]) ^ 2 },
  gr = function(x) { c(-400 * x[1] * (x[2] - x[1] * x[1]) - 2 * (1 - x[1]),
    200 * (x[2] - x[1] * x[1])) }
)
rb0 <- c(-1.2, 1)

# Create an optimizer and initialize it for use with the Rosenbrock function
opt <- make_mize(method = "L-BFGS", par = rb0, fg = rosenbrock_fg)

# Create optimizer without initialization
opt <- make_mize(method = "L-BFGS")

# Need to call mize_init separately:
opt <- mize_init(opt, rb0, rosenbrock_fg)
```

---

**mize**

### Numerical Optimization

**Description**

Numerical optimization including conjugate gradient, Broyden-Fletcher-Goldfarb-Shanno (BFGS), and the limited memory BFGS.

**Usage**

```r
mize(par, fg, method = "L-BFGS", norm_direction = FALSE, memory = 5,
    scale_hess = TRUE, cg_update = "PR+", preconditioner = "",
    tn_init = 0, tn_exit = "curvature", nest_q = 0,
    nest_convex_approx = FALSE, nest_burn_in = 0, step_up = 1.1,
    step_up_fun = "x", step_down = NULL, dbd_weight = 0.1,
    line_search = "More-Thuente", c1 = 1e-04, c2 = NULL,
    step0 = NULL, step_next_init = NULL, try_newton_step = NULL
```
mize

ls_max_fn = 20, ls_max_gr = Inf, ls_max_fg = Inf,
ls_max_alpha_mult = Inf, ls_max_alpha = Inf, ls_safe_cubic = FALSE,
strong_curvature = NULL, approx_armijo = NULL, mom_type = NULL,
mom_schedule = NULL, mom_init = NULL, mom_final = NULL,
mom_switch_iter = NULL, mom_linear_weight = FALSE,
use_init_mom = FALSE, restart = NULL, restart_wait = 10,
max_iter = 100, max_fn = Inf, max_gr = Inf, max_fg = Inf,
abs_tol = sqrt(.Machine$double.eps), rel_tol = abs_tol,
grad_tol = NULL, ginf_tol = NULL,
step_tol = sqrt(.Machine$double.eps), check_conv_every = 1,
log_every = check_conv_every, verbose = FALSE,
store_progress = FALSE)

Arguments

par Initial values for the function to be optimized over.
fg Function and gradient list. See 'Details'.
method Optimization method. See 'Details'.
norm_direction If TRUE, then the steepest descent direction is normalized to unit length. Useful
for adaptive step size methods where the previous step size is used to initialize
the next iteration.
memory The number of updates to store if using the L-BFGS method. Ignored otherwise.
Must be a positive integer.
scale_hess if TRUE, the approximation to the inverse Hessian is scaled according to the
method described by Nocedal and Wright (approximating an eigenvalue). Applies
only to the methods BFGS (where the scaling is applied only during the first
step) and L-BFGS (where the scaling is applied during every iteration). Ignored
otherwise.
cg_update Type of update to use for the "CG" method. For details see the "CG" subsection
of the "Optimization Methods" section. Ignored if method is not "CG".
preconditioner Type of preconditioner to use in Truncated Newton. Leave blank or set to
"L-BFGS" to use a limited memory BFGS preconditioner. Use the "memory" pa-
rameter to control the number of updates to store. Applies only if method = "TN"
or "CG", ignored otherwise.
tn_init Type of initialization to use in inner loop of Truncated Newton. Use 0 to use the
zero vector (the usual TN initialization), or "previous" to use the final result
from the previous iteration, as suggested by Martens (2010). Applies only if
method = "TN", ignored otherwise.
tn_exit Type of exit criterion to use when terminating the inner CG loop of Truncated
Newton method. Either "curvature" to use the standard negative curvature
test, or "strong" to use the modified "strong" curvature test in TNPACK (Xie
and Schlick, 1999). Applies only if method = "TN", ignored otherwise.
nest_q Strong convexity parameter for the NAG momentum term. Must take a value
between 0 (strongly convex) and 1 (zero momentum). Only applies using the
NAG method or a momentum method with Nesterov momentum schedule. Also
does nothing if nest_convex_approx is TRUE.
If `TRUE`, then use an approximation due to Sutskever for calculating the momentum parameter in the NAG method. Only applies using the NAG method or a momentum method with Nesterov momentum schedule.

Number of iterations to wait before using a non-zero momentum. Only applies using the NAG method or a momentum method with Nesterov momentum schedule.

Value by which to increase the step size for the "bold" step size method or the "DBD" method.

Operator to use when combining the current step size with `step_up`. Can be one of "*" (to multiply the current step size with `step_up`) or "+" (to add).

Multiplier to reduce the step size by if using the "DBD" method or the "bold" line search method. Should be a positive value less than 1. Also optional for use with the "back" line search method.

Weighting parameter used by the "DBD" method only, and only if no momentum scheme is provided. Must be an integer between 0 and 1.

Type of line search to use. See 'Details'.

Sufficient decrease parameter for Wolfe-type line searches. Should be a value between 0 and 1.

Sufficient curvature parameter for line search for Wolfe-type line searches. Should be a value between `c1` and 1.

Initial value for the line search on the first step. See 'Details'.

For Wolfe-type line searches only, try the line step value of 1 as the initial step size whenever `step_next_init` suggests a step size > 1. Defaults to `TRUE` for quasi-Newton methods such as BFGS and L-BFGS, `FALSE` otherwise.

Maximum number of function evaluations allowed during a line search.

Maximum number of gradient evaluations allowed during a line search.

Maximum number of function or gradient evaluations allowed during a line search.

The maximum value that can be attained by the ratio of the initial guess for alpha for the current line search, to the final value of alpha of the previous line search. Used to stop line searches diverging due to very large initial guesses. Only applies for Wolfe-type line searches.

Maximum value of alpha allowed during line search. Only applies for `line_search = "more-thuente"`.

(Optional). If `TRUE`, check that cubic interpolation in the Wolfe line search does not produce too small a value, using method of Xie and Schlick (2002). Only applies for `line_search = "more-thuente"`.

(Optional). If `TRUE` use the strong curvature condition in Wolfe line search. See the 'Line Search' section for details.
approx_armijo (Optional). If TRUE use the approximate Armijo condition in Wolfe line search. See the 'Line Search' section for details.
mom_type Momentum type, either "classical" or "nesterov". See 'Details'.
mom_schedule Momentum schedule. See 'Details'.
mom_init Initial momentum value.
mom_final Final momentum value.
mom_switch_iter For mom_schedule "switch" only, the iteration when mom_init is changed to mom_final.
mom_linear_weight If TRUE, the gradient contribution to the update is weighted using momentum contribution.
use_init_mom If TRUE, then the momentum coefficient on the first iteration is non-zero. Otherwise, it's zero. Only applies if using a momentum schedule.
restart Momentum restart type. Can be one of "fn", "gr" or "speed". See 'Details'. Ignored if no momentum scheme is being used.
restart_wait Number of iterations to wait between restarts. Ignored if restart is NULL.
max_iter Maximum number of iterations to optimize for. Defaults to 100. See the 'Convergence' section for details.
max_fn Maximum number of function evaluations. See the 'Convergence' section for details.
max_gr Maximum number of gradient evaluations. See the 'Convergence' section for details.
max_fg Maximum number of function or gradient evaluations. See the 'Convergence' section for details.
abs_tol Absolute tolerance for comparing two function evaluations. See the 'Convergence' section for details.
rel_tol Relative tolerance for comparing two function evaluations. See the 'Convergence' section for details.
grad_tol Absolute tolerance for the length (l2-norm) of the gradient vector. See the 'Convergence' section for details.
ginf_tol Absolute tolerance for the infinity norm (maximum absolute component) of the gradient vector. See the 'Convergence' section for details.
step_tol Absolute tolerance for the size of the parameter update. See the 'Convergence' section for details.
check_conv_every Positive integer indicating how often to check convergence. Default is 1, i.e. every iteration. See the 'Convergence' section for details.
log_every Positive integer indicating how often to log convergence results to the console. Ignored if verbose is FALSE. If not an integer multiple of check_conv_every, it will be set to check_conv_every.
verbose If TRUE, log information about the progress of the optimization to the console.
store_progress If TRUE store information about the progress of the optimization in a data frame, and include it as part of the return value.
Details

The function to be optimized should be passed as a list to the \texttt{fg} parameter. This should consist of:

- \texttt{fn}. The function to be optimized. Takes a vector of parameters and returns a scalar.
- \texttt{gr}. The gradient of the function. Takes a vector of parameters and returns a vector with the same length as the input parameter vector.
- \texttt{fg}. (Optional) function which calculates the function and gradient in the same routine. Takes a vector of parameters and returns a list containing the function result as \texttt{fn} and the gradient result as \texttt{gr}.
- \texttt{hs}. (Optional) Hessian of the function. Takes a vector of parameters and returns a square matrix with dimensions the same as the length of the input vector, containing the second derivatives. Only required to be present if using the "NEWTON" method. If present, it will be used during initialization for the "BFGS" and "SR1" quasi-Newton methods (otherwise, they will use the identity matrix). The quasi-Newton methods are implemented using the inverse of the Hessian, and rather than directly invert the provided Hessian matrix, will use the inverse of the diagonal of the provided Hessian only.

The \texttt{fg} function is optional, but for some methods (e.g. line search methods based on the Wolfe criteria), both the function and gradient values are needed for the same parameter value. Calculating them in the same function can save time if there is a lot of shared work.

Value

A list with components:

- \texttt{par} Optimized parameters. Normally, this is the best set of parameters seen during optimization, i.e. the set that produced the minimum function value. This requires that convergence checking with is carried out, including function evaluation where necessary. See the 'Convergence' section for details.
- \texttt{nf} Total number of function evaluations carried out. This includes any extra evaluations required for convergence calculations. Also, a function evaluation may be required to calculate the value of \texttt{f} returned in this list (see below). Additionally, if the \texttt{verbose} parameter is \texttt{TRUE}, then function and gradient information for the initial value of \texttt{par} will be logged to the console. These values are cached for subsequent use by the optimizer.
- \texttt{ng} Total number of gradient evaluations carried out. This includes any extra evaluations required for convergence calculations using \texttt{grad_tol}. As with \texttt{nf}, additional gradient calculations beyond what you’re expecting may have been needed for logging, convergence and calculating the value of \texttt{g2} or \texttt{ginf} (see below).
- \texttt{f} Value of the function, evaluated at the returned value of \texttt{par}.
- \texttt{g2} Optional: the length (Euclidean or l2-norm) of the gradient vector, evaluated at the returned value of \texttt{par}. Calculated only if \texttt{grad_tol} is non-null.
- \texttt{ginf} Optional: the infinity norm (maximum absolute component) of the gradient vector, evaluated at the returned value of \texttt{par}. Calculated only if \texttt{g1nf_tol} is non-null.
- \texttt{iter} The number of iterations the optimization was carried out for.
- \texttt{terminate} List containing items: \texttt{what}, indicating what convergence criterion was met, and \texttt{val} specifying the value at convergence. See the 'Convergence' section for more details.
• progress Optional data frame containing information on the value of the function, gradient, momentum, and step sizes evaluated at each iteration where convergence is checked. Only present if store_progress is set to TRUE. Could get quite large if the optimization is long and the convergence is checked regularly.

Optimization Methods

The method specifies the optimization method:

• "SD" is plain steepest descent. Not very effective on its own, but can be combined with various momentum approaches.
• "BFGS" is the Brodyen-Fletcher-Goldfarb-Shanno quasi-Newton method. This stores an approximation to the inverse of the Hessian of the function being minimized, which requires storage proportional to the square of the length of par, so is unsuitable for large problems.
• "SR1" is the Symmetric Rank 1 quasi-Newton method, incorporating the safeguard given by Nocedal and Wright. Even with the safeguard, the SR1 method is not guaranteed to produce a descent direction. If this happens, the BFGS update is used for that iteration instead. Note that I have not done any research into the theoretical justification for combining BFGS with SR1 like this, but empirically (comparing to BFGS results with the datasets in the unconstrn package httpsZOOgithubNcomOjlmelvilleOfunconstrain), it works competitively with BFGS, particularly with a loose line search.
• "L-BFGS" is the Limited memory Brodyen-Fletcher-Goldfarb-Shanno quasi-Newton method. This does not store the inverse Hessian approximation directly and so can scale to larger-sized problems than "BFGS". The amount of memory used can be controlled with the memory parameter.
• "CG" is the conjugate gradient method. The cg_update parameter allows for different methods for choosing the next direction:
  - "FR" The method of Fletcher and Reeves.
  - "PR" The method of Polak and Ribiere.
  - "PR+" The method of Polak and Ribiere with a restart to steepest descent if conjugacy is lost. The default.
  - "HS" The method of Hestenes and Stiefel.
  - "DY" The method of Dai and Yuan.
  - "HZ" The method of Hager and Zhang.
  - "HZ+" The method of Hager and Zhang with restart, as used in CG_DESCENT.

The "PR+" and "HZ+" are likely to be most robust in practice. Other updates are available more for curiosity purposes.
• "TN" is the Truncated Newton method, which approximately solves the Newton step without explicitly calculating the Hessian (at the expense of extra gradient calculations).
• "NAG" is the Nesterov Accelerated Gradient method. The exact form of the momentum update in this method can be controlled with the following parameters:
  - nest_q Strong convexity parameter. Must take a value between 0 (strongly convex) and 1 (zero momentum). Ignored if nest_convex_approx is TRUE.
- `nest_convex_approx` If TRUE, then use an approximation due to Sutskever for calculating the momentum parameter.
- `nest_burn_in` Number of iterations to wait before using a non-zero momentum.

- "DBD" is the Delta-Bar-Delta method of Jacobs.
- "Momentum" is steepest descent with momentum. See below for momentum options.

For more details on gradient-based optimization in general, and the BFGS, L-BFGS and CG methods, see Nocedal and Wright.

**Line Search**

The parameter `line_search` determines the line search to be carried out:

- "Rasmussen" carries out a line search using the strong Wolfe conditions as implemented by Carl Edward Rasmussen's minimize.m routines.
- "More-Thuente" carries out a line search using the strong Wolfe conditions and the method of More-Thuente. Can be abbreviated to "MT".
- "Schmidt" carries out a line search using the strong Wolfe conditions as implemented in Mark Schmidt's minFunc routines.
- "Backtracking" carries out a back tracking line search using the sufficient decrease (Armijo) condition. By default, cubic interpolation is used to find an acceptable step size. A constant step size reduction can be used by specifying a value for `step_down` between 0 and 1 (e.g. step size will be halved if `step_down` is set to 0.5).
- "Bold Driver" carries out a back tracking line search until a reduction in the function value is found.
- "Constant" uses a constant line search, the value of which should be provided with `step0`. Note that this value will be multiplied by the magnitude of the direction vector used in the gradient descent method. For method "SD" only, setting the `norm_direction` parameter to TRUE will scale the direction vector so it has unit length.

If using one of the methods: "BFGS", "L-BFGS", "CG" or "NAG", one of the Wolfe line searches: "Rasmussen" or "More-Thuente", "Schmidt" or "Hager-Zhang" should be used, otherwise very poor performance is likely to be encountered. The following parameters can be used to control the line search:

- `c1` The sufficient decrease condition. Normally left at its default value of 1e-4.
- `c2` The sufficient curvature condition. Defaults to 0.9 if using the methods "BFGS" and "L-BFGS", and to 0.1 for every other method, more or less in line with the recommendations given by Nocedal and Wright. The smaller the value of `c2`, the stricter the line search, but it should not be set to smaller than `c1`.
- `step0` Initial value for the line search on the first step. If a positive numeric value is passed as an argument, that value is used as-is. Otherwise, by passing a string as an argument, a guess is made based on values of the gradient, function or parameters, at the starting point:
  - "rasmussen" As used by Rasmussen in minimize.m:
    \[
    \frac{1}{1 + |g|^2}
    \]
- "scipy" As used in optimize.py in the python library Scipy.

\[
\frac{1}{|g|}
\]

- "schmidt" As used by Schmidt in minFunc.m (the reciprocal of the l1 norm of g)

\[
\frac{1}{|g|_1}
\]

- "hz" The method suggested by Hager and Zhang (2006) for the CG_DESCENT software.

These arguments can be abbreviated.

• **step_next_init** How to initialize alpha value of subsequent line searches after the first, using results from the previous line search:
  - "slope ratio" Slope ratio method.
  - "quadratic" Quadratic interpolation method.
  - scalar numeric Set to a numeric value (e.g. step_next_init = 1) to explicitly set alpha to this value initially.

These arguments can be abbreviated. Details on the first two methods are provided by Nocedal and Wright.

• **try_newton_step** For quasi-Newton methods (e.g. "TN", "BFGS" and "L-BFGS"), setting this to TRUE will try the "natural" step size of 1, whenever the step_next_init method suggests an initial step size larger than that.

• **strong_curvature** If TRUE, then the strong curvature condition will be used to check termination in Wolfe line search methods. If FALSE, then the standard curvature condition will be used. The default is NULL which lets the different Wolfe line searches choose whichever is their default behavior. This option is ignored if not using a Wolfe line search method.

• **approx_armijo** If TRUE, then the approximate Armijo sufficient decrease condition (Hager and Zhang, 2005) will be used to check termination in Wolfe line search methods. If FALSE, then the exact curvature condition will be used. The default is NULL which lets the different Wolfe line searches choose whichever is their default behavior. This option is ignored if not using a Wolfe line search method.

For the Wolfe line searches, the methods of "Rasmussen", "Schmidt" and "More-Thuente" default to using the strong curvature condition and the exact Armijo condition to terminate the line search (i.e. Strong Wolfe conditions). The default step size initialization methods use the Rasmussen method for the first iteration and quadratic interpolation for subsequent iterations.

The "Hager-Zhang" Wolfe line search method defaults to the standard curvature condition and the approximate Armijo condition (i.e. approximate Wolfe conditions). The default step size initialization methods are those used by Hager and Zhang (2006) in the description of CG_DESCENT.

If the "DBD" is used for the optimization "method", then the line_search parameter is ignored, because this method controls both the direction of the search and the step size simultaneously. The following parameters can be used to control the step size:

• **step_up** The amount by which to increase the step size in a direction where the current step size is deemed to be too short. This should be a positive scalar.
• `step_down` The amount by which to decrease the step size in a direction where the currents step size is deemed to be too long. This should be a positive scalar smaller than 1. Default is 0.5.

• `step_up_fun` How to increase the step size: either the method of Jacobs (addition of `step_up`) or Janet and co-workers (multiplication by `step_up`). Note that the step size decrease `step_down` is always a multiplication.

The "bold driver" line search also uses the `step_up` and `step_down` parameters with similar meanings to their use with the "DBD" method: the backtracking portion reduces the step size by a factor of `step_down`. Once a satisfactory step size has been found, the line search for the next iteration is initialized by multiplying the previously found step size by `step_up`.

### Momentum

For method "Momentum", momentum schemes can be accessed through the momentum arguments:

• `mom_type` Momentum type, either "classical" or "nesterov" (case insensitive, can be abbreviated). Using "nesterov" applies the momentum step before the gradient descent as suggested by Sutskever, emulating the behavior of the Nesterov Accelerated Gradient method.

• `mom_schedule` How the momentum changes over the course of the optimization:
  - If a numerical scalar is provided, a constant momentum will be applied throughout.
  - "nsconvex" Use the momentum schedule from the Nesterov Accelerated Gradient method suggested for non-strongly convex functions. Parameters which control the NAG momentum can also be used in combination with this option.
  - "switch" Switch from one momentum value (specified via `mom_init`) to another (`mom_final`) at a a specified iteration (`mom_switch_iter`).
  - "ramp" Linearly increase from one momentum value (`mom_init`) to another (`mom_final`).
  - If a function is provided, this will be invoked to provide a momentum value. It must take one argument (the current iteration number) and return a scalar.

String arguments are case insensitive and can be abbreviated.

The restart parameter provides a way to restart the momentum if the optimization appears to be not be making progress, inspired by the method of O’Donoghue and Candes (2013) and Su and co-workers (2014). There are three strategies:

• "fn" A restart is applied if the function does not decrease on consecutive iterations.
• "gr" A restart is applied if the direction of the optimization is not a descent direction.
• "speed" A restart is applied if the update vector is not longer (as measured by Euclidean 2-norm) in consecutive iterations.

The effect of the restart is to "forget" any previous momentum update vector, and, for those momentum schemes that change with iteration number, to effectively reset the iteration number back to zero. If the `mom_type` is "nesterov", the gradient-based restart is not available. The `restart_wait` parameter controls how many iterations to wait after a restart, before allowing another restart. Must be a positive integer. Default is 10, as used by Su and co-workers (2014). Setting this too low could cause premature convergence. These methods were developed specifically for the NAG method, but can be employed with any momentum type and schedule.

If method type "momentum" is specified with no other values, the momentum scheme will default to a constant value of 0.9.
Convergence

There are several ways for the optimization to terminate. The type of termination is communicated by a two-item list terminate in the return value, consisting of what, a short string describing what caused the termination, and val, the value of the termination criterion that caused termination.

The following parameters control various stopping criteria:

- **max_iter** Maximum number of iterations to calculate. Reaching this limit is indicated by terminate$what being "max_iter".
- **max_fn** Maximum number of function evaluations allowed. Indicated by terminate$what being "max_fn".
- **max_gr** Maximum number of gradient evaluations allowed. Indicated by terminate$what being "max_gr".
- **max_fg** Maximum number of gradient evaluations allowed. Indicated by terminate$what being "max_fg".
- **abs_tol** Absolute tolerance of the function value. If the absolute value of the function falls below this threshold, terminate$what will be "abs_tol". Will only be triggered if the objective function has a minimum value of zero.
- **rel_tol** Relative tolerance of the function value, comparing consecutive function evaluation results. Indicated by terminate$what being "rel_tol".
- **grad_tol** Absolute tolerance of the l2 (Euclidean) norm of the gradient. Indicated by terminate$what being "grad_tol". Note that the gradient norm is not a very reliable stopping criterion (see Nocedal and co-workers 2002), but is quite commonly used, so this might be useful for comparison with results from other optimization software.
- **ginf_tol** Absolute tolerance of the infinity norm (maximum absolute component) of the gradient. Indicated by terminate$what being "ginf_tol".
- **step_tol** Absolute tolerance of the step size, i.e. the Euclidean distance between values of par fell below the specified value. Indicated by terminate$what being "step_tol". For those optimization methods which allow for abandoning the result of an iteration and restarting using the previous iteration’s value of par an iteration, step_tol will not be triggered.

Convergence is checked between specific iterations. How often is determined by the check_conv_every parameter, which specifies the number of iterations between each check. By default, this is set for every iteration.

Be aware that if abs_tol or rel_tol are non-NULL, this requires the function to have been evaluated at the current position at the end of each iteration. If the function at that position has not been calculated, it will be calculated and will contribute to the total reported in the courts list in the return value. The calculated function value is cached for use by the optimizer in the next iteration, so if the optimizer would have needed to calculate the function anyway (e.g. use of the strong Wolfe line search methods), there is no significant cost accrued by calculating it earlier for convergence calculations. However, for methods that don’t use the function value at that location, this could represent a lot of extra function evaluations. On the other hand, not checking convergence could result in a lot of extra unnecessary iterations. Similarly, if grad_tol or ginf_tol is non-NULL, then the gradient will be calculated if needed.

If extra function or gradient evaluations is an issue, set check_conv_every to a higher value, but be aware that this can cause convergence limits to be exceeded by a greater amount.
Note also that if the verbose parameter is True, then a summary of the results so far will be logged to the console whenever a convergence check is carried out. If the store_progress parameter is True, then the same information will be returned as a data frame in the return value. For a long optimization this could be a lot of data, so by default it is not stored.

Other ways for the optimization to terminate is if an iteration generates a non-finite (i.e. Inf or NaN) gradient or function value. Some, but not all, line-searches will try to recover from the latter, by reducing the step size, but a non-finite gradient calculation during the gradient descent portion of optimization is considered catastrophic by mize, and it will give up. Termination under non-finite gradient or function conditions will result in terminate what being "gr_inf" or "fn_inf" respectively. Unlike the convergence criteria, the optimization will detect these error conditions and terminate even if a convergence check would not be carried out for this iteration.

The value of par in the return value should be the parameters which correspond to the lowest value of the function that has been calculated during the optimization. As discussed above however, determining which set of parameters requires a function evaluation at the end of each iteration, which only happens if either the optimization method calculates it as part of its own operation or if a convergence check is being carried out during this iteration. Therefore, if your method does not carry out function evaluations and check_conv_every is set to be so large that no convergence calculation is carried out before max_iter is reached, then the returned value of par is the last value encountered.

References


**Examples**

```r
# Function to optimize and starting point defined after creating optimizer
rosenbrock_fg <- list(
  fn = function(x) { 100 * (x[2] - x[1] * x[1]) ^ 2 + (1 - x[1]) ^ 2 },
)
rb0 <- c(-1.2, 1)

# Minimize using L-BFGS
res <- mize(rb0, rosenbrock_fg, method = "L-BFGS")

# Conjugate gradient with Fletcher-Reeves update, tight Wolfe line search
res <- mize(rb0, rosenbrock_fg, method = "CG", cg_update = "FR", c2 = 0.1)

# Steepest decent with constant momentum = 0.9
res <- mize(rb0, rosenbrock_fg, method = "MOM", mom_schedule = 0.9)

# Steepest descent with constant momentum in the Nesterov style as described in papers by Sutskever and Bengio
res <- mize(rb0, rosenbrock_fg, method = "MOM", mom_type = "nesterov", mom_schedule = 0.9)

# Nesterov momentum with adaptive restart comparing function values
res <- mize(rb0, rosenbrock_fg, method = "MOM", mom_type = "nesterov", mom_schedule = 0.9, restart = "fn")
```

### Description

Prepares the optimizer for use with a specific function and starting point.
Usage

\[ \text{mize_init}(\text{opt, par, fg, max\_iter = Inf, max\_fn = Inf, max\_gr = Inf, max\_fg = Inf, abs\_tol = NULL, rel\_tol = abs\_tol, grad\_tol = NULL, ginf\_tol = NULL, step\_tol = NULL)} \]

Arguments

- \text{opt} \quad \text{Optimizer, created by make_mize.}
- \text{par} \quad \text{Vector of initial values for the function to be optimized over.}
- \text{fg} \quad \text{Function and gradient list. See the documentation of mize.}
- \text{max\_iter} \quad \text{(Optional). Maximum number of iterations. See the 'Convergence' section of mize for details.}
- \text{max\_fn} \quad \text{(Optional). Maximum number of function evaluations. See the 'Convergence' section of mize for details.}
- \text{max\_gr} \quad \text{(Optional). Maximum number of gradient evaluations. See the 'Convergence' section of mize for details.}
- \text{max\_fg} \quad \text{(Optional). Maximum number of function or gradient evaluations. See the 'Convergence' section of mize for details.}
- \text{abs\_tol} \quad \text{(Optional). Absolute tolerance for comparing two function evaluations. See the 'Convergence' section of mize for details.}
- \text{rel\_tol} \quad \text{(Optional). Relative tolerance for comparing two function evaluations. See the 'Convergence' section of mize for details.}
- \text{grad\_tol} \quad \text{(Optional). Absolute tolerance for the length (l2-norm) of the gradient vector. See the 'Convergence' section of mize for details.}
- \text{ginf\_tol} \quad \text{(Optional). Absolute tolerance for the infinity norm (maximum absolute component) of the gradient vector. See the 'Convergence' section of mize for details.}
- \text{step\_tol} \quad \text{(Optional). Absolute tolerance for the size of the parameter update. See the 'Convergence' section of mize for details.}

Details

Should be called after creating an optimizer with make_mize and before beginning any optimization with mize_step. Note that if \text{fg} and \text{par} are available at the time mize_step is called, they can be passed to that function and initialization will be carried out automatically, avoiding the need to call mize_init.

Optional convergence parameters may also be passed here, for use with check_mize_convergence. They are optional if you do your own convergence checking.

Details of the \text{fg} list can be found in the 'Details' section of mize.

Value

- Initialized optimizer.
Examples

```r
# Create an optimizer
opt <- make_mize(method = "L-BFGS")

# Function to optimize and starting point defined after creating optimizer
rosenbrook_fg <- list(
  fn = function(x) { 100 * (x[2] - x[1] * x[1]) ^ 2 + (1 - x[1]) ^ 2 },
  gr = function(x) { c(-400 * x[1] * (x[2] - x[1] * x[1]) - 2 * (1 - x[1]),

rb0 <- c(-1.2, 1)

# Initialize with function and starting point before commencing optimization
opt <- mize_init(opt, rb0, rosenbrook_fg)

# Finally, can commence the optimization loop
par <- rb0
for (iter in 1:3) {
  res <- mize_step(opt, par, rosenbrook_fg)
  par <- res$par
  opt <- res$opt
}
```

---

**mize_step**

*One Step of Optimization*

**Description**

Performs one iteration of optimization using a specified optimizer.

**Usage**

```r
mize_step(opt, par, fg)
```

**Arguments**

- `opt` Optimizer, created by `make_mize`.
- `par` Vector of initial values for the function to be optimized over.
- `fg` Function and gradient list. See the documentation of `mize`.

**Details**

This function returns both the (hopefully) optimized vector of parameters, and an updated version of the optimizer itself. This is intended to be used when you want more control over the optimization process compared to the more black box approach of the `mize` function. In return for having to manually call this function every time you want the next iteration of optimization, you gain the
ability to do your own checks for convergence, logging and so on, as well as take other action between iterations, e.g. visualization.

Normally calling this function should return a more optimized vector of parameters than the input, or at least leave the parameters unchanged if no improvement was found, although this is determined by how the optimizer was configured by `make_mize`. It is very possible to create an optimizer that can cause a solution to diverge. It is the responsibility of the caller to check that the result of the optimization step has actually reduced the value returned from function being optimized.

Details of the `fg` list can be found in the 'Details' section of `mize`.

**Value**

Result of the current optimization step, a list with components:

- **opt.** Updated version of the optimizer passed to the `opt` argument. Should be passed as the `opt` argument in the next iteration.
- **par.** Updated version of the parameters passed to the `par` argument. Should be passed as the `par` argument in the next iteration.
- **nf.** Running total number of function evaluations carried out since iteration 1.
- **ng.** Running total number of gradient evaluations carried out since iteration 1.
- **f.** Optional. The new value of the function, evaluated at the returned value of `par`. Only present if calculated as part of the optimization step (e.g. during a line search calculation).
- **g.** Optional. The gradient vector, evaluated at the returned value of `par`. Only present if the gradient was calculated as part of the optimization step (e.g. during a line search calculation.)

**See Also**

`make_mize` to create a value to pass to `opt`, `mize_init` to initialize `opt` before passing it to this function for the first time. `mize` creates an optimizer and carries out a full optimization with it.

**Examples**

```r
rosenbrock_fg <- list(
  fn = function(x) {
    100 * (x[2] - x[1] * x[1])^2 + (1 - x[1])^2
  },
  gr = function(x) {
    c(
  })
rb0 <- c(-1.2, 1)

opt <- make_mize(method = "SD", line_search = "const", step0 = 0.0001,
                  par = rb0, fg = rosenbrock_fg)
par <- rb0
for (iter in 1:3) {
  res <- mize_step(opt, par, rosenbrock_fg)
  par <- res$par
  opt <- res$opt
}
```
Mize Step Summary

Description

Produces a result summary for an optimization iteration. Information such as function value, gradient norm and step size may be returned.

Usage

mize_step_summary(opt, par, fg, par_old = NULL, calc_fn = NULL)

Arguments

opt Optimizer to generate summary for, from return value of mize_step.
par Vector of parameters at the end of the iteration, from return value of mize_step.
fg Function and gradient list. See the documentation of mize.
par_old (Optional). Vector of parameters at the end of the previous iteration. Used to calculate step size.
calc_fn (Optional). If TRUE, force calculation of function if not already cached in opt, even if it would not be needed for convergence checking.

Details

By default, convergence tolerance parameters will be used to determine what function and gradient data is returned. The function value will be returned if it was already calculated and cached in the optimization iteration. Otherwise, it will be calculated only if a non-null absolute or relative tolerance value was asked for. A gradient norm will be returned only if a non-null gradient tolerance was specified, even if the gradient is available.

Note that if a function tolerance was specified, but was not calculated for the relevant value of par, they will be calculated here and the calculation does contribute to the total function count (and will be cached for potential use in the next iteration). The same applies for gradient tolerances and gradient calculation. Function and gradient calculation can also be forced here by setting the calc_fn and calc_gr (respectively) parameters to TRUE.

Value

A list with the following items:

- opt Optimizer with updated state (e.g. function and gradient counts).
- iter Iteration number.
- f Function value at par.
- g2n 2-norm of the gradient at par.
- ginfn Infinity-norm of the gradient at par.
- nf Number of function evaluations so far.
• Number of gradient evaluations so far.
• Step Size of the step between \( \text{par}_\text{old} \) and \( \text{par} \), if \( \text{par}_\text{old} \) is provided.
• \( \alpha \) Step length of the gradient descent part of the step.
• \( \mu \) Momentum coefficient for this iteration

Examples

```r
rb_fg <- list(
  fn = function(x) { 100 * (x[2] - x[1] * x[1])^2 + (1 - x[1])^2 },
  gr = function(x) { c(-400 * x[1] * (x[2] - x[1] * x[1]),
rb0 <- c(-1.2, 1)

opt <- make_mize(method = "BFGS", par = rb0, fg = rb_fg, max_iter = 30)
mize_res <- mize_step(opt = opt, par = rb0, fg = rb_fg)
# Get info about first step, use rb0 to compare new par with initial value
step_info <- mize_step_summary(mize_res$opt, mize_res$par, rb_fg, rb0)
```
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