Package 'ucminf'

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Title General-Purpose Unconstrained Non-Linear Optimization

Version 1.2.2

Description An algorithm for general-purpose unconstrained non-linear optimization. The algorithm is of quasi-Newton type with BFGS updating of the inverse Hessian and soft line search with a trust region type monitoring of the input to the line search algorithm. The interface of 'ucminf' is designed for easy interchange with 'optim'.

License GPL (>= 2)

URL https://github.com/hdakpo/ucminf

BugReports https://github.com/hdakpo/ucminf/issues

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Depends R (>= 3.5.0)

Suggests numDeriv

NeedsCompilation yes

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Contents

ucminf-package						•	•	•			•	•	•	•			•		•	•		•			•	•	•		•		•		•			2
ucminf	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•		•	•	•	•	•	•	•	2

6

Index

ucminf-package

Description

The ucminf package provides an algorithm for general-purpose unconstrained non-linear optimization.

Bugreport

Any bug or suggestion can be reported using the ucminf tracker facilities at: https://github. com/hdakpo/ucminf/issues

Author(s)

K Hervé Dakpo, Hans Bruun Nielsen, and Stig Bousgaard Mortensen

ucminf

General-Purpose Unconstrained Non-Linear Optimization

Description

An algorithm for general-purpose unconstrained non-linear optimization. The algorithm is of quasi-Newton type with BFGS updating of the inverse Hessian and soft line search with a trust region type monitoring of the input to the line search algorithm. The interface of 'ucminf' is designed for easy interchange with 'optim'.

Usage

ucminf(par, fn, gr = NULL, ..., control = list(), hessian = 0)

Arguments

par	Initial estimate of minimum for fn.
fn	Objective function to be minimized.
gr	Gradient of objective function. If NULL a finite difference approximation is used.
	Optional arguments passed to the objective and gradient functions.
control	A list of control parameters. See 'Details'.
hessian	Integer value:
	0 No hessian approximation is returned.
	1 Returns a numerical approximation of the Hessian using 'hessian' in the pack- age 'numDeriv'.
	2 Returns final approximation of the inverse Hessian based on the series of BFGS updates during optimization.
	3 Same at 2, but will also return the Hessian (the inverse of 2).
	If a TRUE or FALSE value is given it will switch between option 1 or 0.

ucminf

Details

The algorithm is documented in (Nielsen, 2000) (see References below) together with a comparison to the Fortran subroutine 'MINF' and the Matlab function 'fminunc'. The implementation of 'ucminf' in R uses the original Fortran version of the algorithm.

The interface in R is designed so that it is very easy to switch between using 'ucminf' and 'optim'. The arguments par, fn, gr, and hessian are all the same (with a few extra options for hessian in 'ucminf'). The difference is that there is no method argument in 'ucminf' and that some of the components in the control argument are different due to differences in the algorithms.

The algorithm can be given an initial estimate of the Hessian for the optimization and it is possible to get the final approximation of the Hessian based on the series of BFGS updates. This extra functionality may be useful for optimization in a series of related problems.

The functions fn and gr can return Inf or NaN if the functions cannot be evaluated at the supplied value, but the functions must be computable at the initial value. The functions are not allowed to return NA. Any names given to par will be copied to the vectors passed to fn and gr. No other attributes of par are copied over.

The control argument is a list that can supply any of the following components:

- trace If trace is positive then detailed tracing information is printed for each iteration.
- grtol The algorithm stops when $||F'(x)||_{\infty} \leq \text{grtol}$, that is when the largest absolute value of the gradient is less than grtol. Default value is grtol = 1e-6.
- xtol The algorithm stops when $||x x_p||_2 \le \text{xtol} \cdot (\text{xtol} + ||x||_2)$, where x_p and x are the previous and current estimate of the minimizer. Thus the algorithm stops when the last relative step length is sufficiently small. Default value is xtol = 1e-12.
- stepmax Initial maximal allowed step length (radius of trust-region). The value is updated during the optimization. Default value is stepmax = 1.
- maxeval The maximum number of function evaluations. A function evaluation is counted as one evaluation of the objective function and of the gradient function. Default value is maxeval = 500.
- grad Either 'forward' or 'central'. Controls the type of finite difference approximation to be used for the gradient if no gradient function is given in the input argument 'gr'. Default value is grad = 'forward'.
- gradstep Vector of length 2. The step length in finite difference approximation for the gradient. Step length is $|x_i| \cdot \text{gradstep}[1]+\text{gradstep}[2]$. Default value is gradstep = c(1e-6, 1e-8).
- invhessian.lt A vector with an initial approximation to the lower triangle of the inverse Hessian. If not given, the inverse Hessian is initialized as the identity matrix. If H0 is the initial hessian matrix then the lower triangle of the inverse of H0 can be found as invhessian.lt = solve(H0)[lower.tri(H0,diag=TRUE)].

Value

ucminf returns a list of class 'ucminf' containing the following elements:

par	Computed minimizer.
value	Objective function value at computed minimizer.
convergence	Flag for reason of termination:

	1 Stopped by small gradient (grtol).
	2 Stopped by small step (xtol).
	3 Stopped by function evaluation limit (maxeval).
	4 Stopped by zero step from line search
	-2 Computation did not start: $length(par) = 0$.
	-4 Computation did not start: stepmax is too small.
	-5 Computation did not start: grtol or xtol ≤ 0 .
	-6 Computation did not start: maxeval <= 0.
	-7 Computation did not start: given Hessian not pos. definite.
message	String with reason of termination.
hessian, invhes	sian
	Estimate of (inv.) Hessian at computed minimizer. The type of estimate is given by the input argument 'hessian'.
invhessian.lt	The lower triangle of the final approximation to the inverse Hessian based on the series of BFGS updates during optimization.
info	Information about the search:
	maxgradient $ F'(x) _{\infty}$, the largest element in the absolute value of the gradient at the computed minimizer.
	laststep Length of last step.
	stepmax Final maximal allowed step length.
	neval Number of calls to both objective and gradient function.

Author(s)

'UCMINF' algorithm design and Fortran code by Hans Bruun Nielsen.

K Hervé Dakpo took over maintenance of the package in May. 2023.

Implementation in R by Stig B. Mortensen, <stigbm@gmail.com>.

Modifications by Douglas Bates <u>bates@stat.wisc.edu</u>, Nov. 2010, to support nested optimization and correct issues with printing on Windows.

References

Nielsen, H. B. (2000) 'UCMINF - An Algorithm For Unconstrained, Nonlinear Optimization', Report IMM-REP-2000-19, Department of Mathematical Modelling, Technical University of Denmark. http://www.imm.dtu.dk/documents/ftp/tr00/tr19_00.pdf

The original Fortran source code was found at http://www2.imm.dtu.dk/projects/hbn_software/ucminf.f. (That URL is no longer available but archived at https://web.archive.org/web/20050418082240/ http://www.imm.dtu.dk/~hbn/Software/ucminf.f - Dr Nielsen passed away in 2015). The code has been slightly modified in this package to be suitable for use with R.

The general structure of the implementation in R is based on the package 'FortranCallsR' by Diethelm Wuertz.

See Also

optim, nlminb, nlm.

ucminf

Examples

Index

nlm,*4* nlminb,*4*

optim, *3*, *4*

ucminf, 2, 3 ucminf-package, 2