Package ‘minqa’

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Type Package

Title Derivative-Free Optimization Algorithms by Quadratic Approximation

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Description Derivative-free optimization by quadratic approximation based on an interface to Fortran implementations by M. J. D. Powell.

License GPL-2

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R topics documented:

bobyqa .................................................... 2
newuoa .................................................. 4
uobyqa ................................................... 6

Index 9
bobyqa

An R interface to the bobyqa implementation of Powell

Description

The purpose of bobyqa is to minimize a function of many variables by a trust region method that forms quadratic models by interpolation. Box constraints (bounds) on the parameters are permitted.

Usage

bobyqa(par, fn, lower = -Inf, upper = Inf, control = list(), ...)

Arguments

par  A numeric vector of starting estimates of the parameters of the objective function.

fn   A function that returns the value of the objective at the supplied set of parameters par using auxiliary data in ... . The first argument of fn must be par.

lower  A numeric vector of lower bounds on the parameters. If the length is 1 the single lower bound is applied to all parameters.

upper A numeric vector of upper bounds on the parameters. If the length is 1 the single upper bound is applied to all parameters.

control  An optional list of control settings. See the details section for the names of the settable control values and their effect.

...  Further arguments to be passed to fn.

Details

The function fn must return a scalar numeric value.

The control argument is a list. Possible named values in the list and their defaults are:

npt  The number of points used to approximate the objective function via a quadratic approximation. The value of npt must be in the interval \([n + 2, (n + 1)(n + 2)/2]\) where \(n\) is the number of parameters in par. Choices that exceed \(2 \times n + 1\) are not recommended. If not defined, it will be set to \(\min(n \times 2, n + 2)\).

rhobeg  rhobeg and rhoend must be set to the initial and final values of a trust region radius, so both must be positive with \(0 < \text{rhoend} < \text{rhobeg}\). Typically rhobeg should be about one tenth of the greatest expected change to a variable. If the user does not provide a value, this will be set to \(\min(0.95, 0.2 \times \max(\text{abs(par}))\). Note also that smallest difference abs(upper-lower) should be greater than or equal to \(\text{rhobeg} \times 2\). If this is not the case then \(\text{rhobeg}\) will be adjusted.

rhoend The smallest value of the trust region radius that is allowed. If not defined, then \(1e-6\) times the value set for rhobeg will be used.
**iprint**  The value of iprint should be set to an integer value in $0, 1, 2, 3, \ldots$, which controls the amount of printing. Specifically, there is no output if iprint=0 and there is output only at the start and the return if iprint=1. Otherwise, each new value of rho is printed, with the best vector of variables so far and the corresponding value of the objective function. Further, each new value of the objective function with its variables are output if iprint=3. If iprint > 3, the objective function value and corresponding variables are output every iprint evaluations. Default value is 0.

**maxfun**  The maximum allowed number of function evaluations. If this is exceeded, the method will terminate.

### Value

A list with components:

- **par**  The best set of parameters found.
- **fval**  The value of the objective at the best set of parameters found.
- **feval**  The number of function evaluations used.
- **ierr**  An integer error code. A value of zero indicates success. Other values are:
  - 1 maximum number of function evaluations exceeded
  - 2 NPT, the number of approximation points, is not in the required interval
  - 3 a trust region step failed to reduce q (Consult Powell for explanation.)
  - 4 one of the box constraint ranges is too small ($< 2*RHOBEG$)
  - 5 bobyqa detected too much cancellation in denominator (We have not fully understood Powell’s code to explain this.)
- **msg**  A message describing the outcome of UOBYQA

### References


Description was taken from comments in the Fortran code of M. J. D. Powell on which minqa is based.

### See Also

- optim, nlminb
Examples

```r
fr <- function(x) { ## Rosenbrock Banana function
    100 * (x[2] - x[1]^-2)^2 + (1 - x[1])^2
}
(x1 <- bobyqa(c(1, 2), fr, lower = c(0, 0), upper = c(4, 4)))
## => optimum at c(1, 1) with fval = 0

str(x1) # see that the error code and msg are returned

# check the error exits
# too many iterations
x1e<-bobyqa(c(1, 2), fr, lower = c(0, 0), upper = c(4, 4), control = list(maxfun=50))
str(x1e)

# Throw an error because bounds too tight
x1b<-bobyqa(c(1, 4), fr, lower = c(0, 3.9999999), upper = c(4, 4))
str(x1b)

# Throw an error because npt is too small -- does NOT work as of 2010-8-10 as
# minqa.R seems to force a reset.
x1n<-bobyqa(c(2,2), fr, lower = c(0, 0), upper = c(4, 4), control=list(npt=1))
str(x1n)

# To add if we can find them -- examples of ierr = 3 and ierr = 5.
```

newuoanewuoaAn R interface to the NEWUOA implementation of Powell

Description

The purpose of newuoa is to minimize a function of many variables by a trust region method that forms quadratic models by interpolation.

Usage

```r
newuoa(par, fn, control = list(), ...)
```

Arguments

- `par` A numeric vector of starting estimates.
- `fn` A function that returns the value of the objective at the supplied set of parameters `par` using auxiliary data in `...`. The first argument of `fn` must be `par`.
- `control` An optional list of control settings. See the details section for the names of the settable control values and their effect.
- `...` Further arguments to be passed to `fn`. 
Details

Functions $fn$ must return a numeric value. The $control$ argument is a list; possible named values in the list and their defaults are:

- **npt** The number of points used to approximate the objective function via a quadratic approximation. The value of npt must be in the interval $[n + 2, (n + 1)(n + 2)/2]$ where $n$ is the number of parameters in $par$. Choices that exceed $2 \times n + 1$ are not recommended. If not defined, it will be set to $\min(n \times 2, n + 2)$.

- **rhobeg** $rhobeg$ and $rhoend$ must be set to the initial and final values of a trust region radius, so both must be positive with $0 < rhoend < rhobeg$. Typically $rhobeg$ should be about one tenth of the greatest expected change to a variable. If the user does not provide a value, this will be set to $\max(par) / 2$.

- **rhoend** The smallest value of the trust region radius that is allowed. If not defined, then $1e-6$ times the value set for $rhobeg$ will be used.

- **iprint** The value of $iprint$ should be set to an integer value in $0, 1, 2, 3, \ldots$, which controls the amount of printing. Specifically, there is no output if $iprint=0$ and there is output only at the start and the return if $iprint=1$. Otherwise, each new value of $rho$ is printed, with the best vector of variables so far and the corresponding value of the objective function. Further, each new value of the objective function with its variables are output if $iprint=3$. If $iprint > 3$, the objective function value and corresponding variables are output every $iprint$ evaluations. Default value is $0$.

- **maxfun** The maximum allowed number of function evaluations. If this is exceeded, the method will terminate.

Value

A list with components:

- **par** The best set of parameters found.
- **fval** The value of the objective at the best set of parameters found.
- **feval** Number of function evaluations to determine the optimum
- **ier** An integer error code. A value of zero indicates success. Other values (consistent with BOBYQA values) are
  1 maximum number of function evaluations exceeded
  2 NPT, the number of approximation points, is not in the required interval
  3 a trust region step failed to reduce $q$ (Consult Powell for explanation.)
  5 newuoa detected too much cancellation in denominator (We have not fully understood Powell’s code to explain this.)
- **msg** A message describing the outcome of UOBYQA

References


Description was taken from comments in the Fortran code of M. J. D. Powell on which minqa is based.

See Also
optim, nlminb

Examples

fr <- function(x) {  
## Rosenbrock Banana function  
  100 * (x[2] - x[1]^2)^2 + (1 - x[1])^2  
}
(x2 <- newuoa(c(1, 2), fr))
## => optimum at c(1, 1) with fval = 0

# check the error exits
# too many iterations
x2e<-newuoa(c(1, 2), fr, control = list(maxfun=50))
str(x2e)

# Throw an error because npt is too small -- does NOT work as of 2010-8-10 as
# minqa.R seems to force a reset.
x2n<-newuoa(c(2,2), fr, control=list(npt=1))
str(x2n)

# To add if we can find them -- examples of ierr = 3 and ierr = 5.

uobyqa

An R interface to the uobyqa implementation of Powell

Description

The purpose of uobyqa is to minimize a function of many variables by a trust region method that forms quadratic models by interpolation.

Usage

uobyqa(par, fn, control = list(), ...)
Arguments

par  A numeric vector of starting estimates.

fn   A function that returns the value of the objective at the supplied set of parameters par using auxiliary data in . . . . The first argument of fn must be par.

control  An optional list of control settings. See the details section for the names of the settable control values and their effect.

. . .  Further arguments to be passed to fn.

Details

Functions fn must return a numeric value.

The control argument is a list. Possible named values in the list and their defaults are:

rhobeg  rhobeg and rhoend must be set to the initial and final values of a trust region radius, so both must be positive with 0 < rhoend < rhobeg. Typically rhobeg should be about one tenth of the greatest expected change to a variable.

rhoend  The smallest value of the trust region radius that is allowed. If not defined, then 1e-6 times the value set for rhobeg will be used.

iprint  The value of iprint should be set to an integer value in 0, 1, 2, 3, . . . , which controls the amount of printing. Specifically, there is no output if iprint=0 and there is output only at the start and the return if iprint=1. Otherwise, each new value of rho is printed, with the best vector of variables so far and the corresponding value of the objective function. Further, each new value of the objective function with its variables are output if iprint=3. If iprint > 3, the objective function value and corresponding variables are output every iprint evaluations. Default value is 0.

maxfun  The maximum allowed number of function evaluations. If this is exceeded, the method will terminate.

Powell’s Fortran code has been slightly modified (thanks to Doug Bates for help on this) to avoid use of PRINT statements. Output is now via calls to C routines set up to work with the routines BOBYQA, NEWUOA and UOBYQA.

Value

A list with components:

par  The best set of parameters found.

fval  The value of the objective at the best set of parameters found.

feval  The number of function evaluations used.

ierr  An integer error code. A value of zero indicates success. Other values (consistent with BOBYQA values) are

1  maximum number of function evaluations exceeded

3  a trust region step failed to reduce q (Consult Powell for explanation.)

msg  A message describing the outcome of UOBYQA
References


Description was taken from comments in the Fortran code of M. J. D. Powell on which minqa is based.

See Also

optim, nlminb

Examples

fr <- function(x) {  ## Rosenbrock Banana function
  100 * (x[2] - x[1]^2)^2 + (1 - x[1])^2
}
(x3 <- uobyqa(c(1, 2), fr))
## => optimum at c(1, 1) with fval = 0

# check the error exits
# too many iterations
x3e <- uobyqa(c(1, 2), fr, control = list(maxfun=50))
str(x3e)

# To add if we can find them -- examples of ierr = 3.
Index

* nonlinear
  bobyqa, 2
  newuoa, 4
  uobyqa, 6

* optimize
  bobyqa, 2
  newuoa, 4
  uobyqa, 6

bobyqa, 2

newuoa, 4

nlminb, 3, 6, 8

optim, 3, 6, 8

uobyqa, 6