Package ‘adagio’

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Description The R package 'adagio' will provide methods and algorithms for
discrete optimization, e.g. knapsack and subset sum procedures,
derivative-free Nelder-Mead and Hooke-Jeeves minimization, and
some (evolutionary) global optimization functions.
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**Description**

Linear (sum) assignment problem, or LSAP.

**Usage**

```r
assignment(cmat, dir = "min")
```

**Arguments**

- `cmat`: quadratic (numeric) matrix, the cost matrix.
- `dir`: direction, can be "min" or "max".

**Details**

Solves the linear (sum) assignment problem for quadratic matrices. Uses the `lp.assign` function from the `lpSolve` package, that is it solves LSAP as a mixed integer linear programming problem.

**Value**

List with components `perm`, the permutation that defines the minimum solution, `min`, the minimum value, and `err` is always 0, i.e. not used at the moment.

**Note**

Slower than the Hungarian algorithm in package `clue`.

**References**

### bpp_approx

**Approximate Bin Packing**

**Description**

Solves the Bin Packing problem approximately.

**Usage**

`bpp_approx(S, cap, method = c("firstfit", "bestfit", "worstfit"))`

**Arguments**

- `S`: vector of weights (or sizes) of items.
- `cap`: same capacity for all the bins.
- `method`: which approximate method to use.

---

### Examples

#### Example similar to clue::solve_LSAP

```r
global::set.seed(8237)
x <- matrix(sample(1:100), nrow = 10)
y <- assignment(x)
  # show permutation and check minimum sum
y$perm # 7 6 10 5 8 2 1 4 9 3
y$min # 173
z <- cbind(1:10, y$perm)
x[z] # 16 9 49 6 17 14 1 44 10 7
y$min == sum(x[z]) # TRUE
```

#### Not run:

---

#### Example: minimize sum of distances of complex points

```r
n <- 100
x <- rt(n, df=3) + 1i * rt(n, df=3)
y <- runif(n) + 1i * runif(n)
cmat <- round(outer(x, y, FUN = function(x,y) Mod(x - y)), 2)
system.time(T1 <- assignment(cmat)) # elapsed: 0.003
T1$min / 100 # 145.75
```

```
## Example: Hungarian algorithm in package 'clue'
library("clue")
system.time(T2 <- solve_LSAP(cmat)) # elapsed: 0.014
sum(cmat[cbind(1:n, T2)]) # 145.75
```

---

### bpp_approx

**Approximate Bin Packing**

**Description**

Solves the Bin Packing problem approximately.

**Usage**

`bpp_approx(S, cap, method = c("firstfit", "bestfit", "worstfit"))`

**Arguments**

- `S`: vector of weights (or sizes) of items.
- `cap`: same capacity for all the bins.
- `method`: which approximate method to use.
Details

Solves approximately the Bin Packing problem for numeric weights and bins, all having the same volume.

Possible methods are "firstfit", "bestfit", and "worstfit". "firstfit" tries to place each item as early as possible, "bestfit" such that the remaining space in the bin is as small as possible, and "worstfit" such that the remaining space is as big as possible.

Best results are achieved with the "bestfit" method. "firstfit" may be a reasonable alternative. For smaller and medium-sized data the approximate results will come quite close to the exact solution, see the examples.

In general, the results are much better if the items in S are sorted decreasingly. If they are not, an immediate warning is issued.

Value

A list of the following components:

- nbins minimum number of bins.
- xbins index of the bin each item is assigned to.
- sbins sum of item sizes in each bin.
- filled total volume filled in the bins (as percentage).

Note

The Bin Packing problem can be solved as a Linear Program. The formulation is a bit tricky, and it turned out 'lpSolve' does not solve medium-sized problems in acceptable time. (Tests with 'Rglpk' will follow.)

Author(s)

Hans W. Borchers

References


See Also

Function `binpacking` in package 'knapsack' (on R-Forge).

Examples

```r
## (1)
S <- c(50, 3, 48, 53, 53, 4, 3, 41, 23, 20, 52, 49)
cap <- 100
bpp_approx(S, cap, method = "bestfit")
## exact -- $nbins 4, filled 99.75 %
## firstfit -- $nbins 6, filled 66.5 %
```
## bestfit -- $nbins 5, filled 79.8 %
## ! when decreasingly sorted, 'bestfit' with nbins = 4

## (2)
S <- c(100,99,89,88,87,75,67,65,65,57,57,49,47,31,27,18,13,9,8,1)
cap <- 100
bpp_approx(S, cap, method = "firstfit")
# firstfit: 12 bins; exact: 12 bins

## Not run:
## (3)
S <- c(99,99,96,92,91,88,87,86,
     85,76,74,72,69,67,67,62,61,56,
     52,51,49,46,44,42,40,40,33,33,
     30,30,29,28,28,27,25,24,23,22,
     21,20,17,14,13,11,10, 7, 7, 3)
cap <- 100
bpp_approx(S, cap)
# exact: 25; firstfit: 25; bestfit: 25 nbins

## (4)
# 20 no.s in 1..100, capacity 100
set.seed(7013)
S <- sample(1:100, 20, replace = TRUE)
cap <- 100
bpp_approx(sort(S, decreasing = TRUE), cap, method = "bestfit")
# exact: 12 bins; firstfit and bestfit: 13; worstfit: 14 bins
## End(Not run)

---

CMAES

**covariance matrix adaptation evolution strategy**

### Description

The CMA-ES (Covariance Matrix Adaptation Evolution Strategy) is an evolutionary algorithm for difficult non-linear non-convex optimization problems in continuous domain. The CMA-ES is typically applied to unconstrained or bounded constraint optimization problems, and search space dimensions between three and fifty.

### Usage

```r
pureCMAES(par, fun, lower = NULL, upper = NULL, sigma = 0.5,
          stopfitness = -Inf, stopeval = 100*length(par)^2, ...)
```

### Arguments

- **par**: objective variables initial point.
- **fun**: objective/target/fitness function.
lower,upper  lower and upper bounds for the parameters.
sigma     coordinate wise standard deviation (step size).
stopfitness stop if fitness < stopfitness (minimization).
stopeval   stop after stopeval number of function evaluations
...       additional parameters to be passed to the function.

Details
The CMA-ES implements a stochastic variable-metric method. In the very particular case of a
convex-quadratic objective function the covariance matrix adapts to the inverse of the Hessian ma-
trix, up to a scalar factor and small random fluctuations. The update equations for mean and covari-
ance matrix maximize a likelihood while resembling an expectation-maximization algorithm.

Value
Returns a list with components xmin and fmin.
Be patient; for difficult problems or high dimensions the function may run for several minutes;
avoid problem dimensions of 30 and more!

Note
There are other implementations of Hansen's CMAES in package 'cmaes' (simplified form) and in
package 'parma' as cmaes() (extended form).

Author(s)
Copyright (c) 2003-2010 Nikolas Hansen for Matlab code PURECMAES; converted to R by Hans
W Borchers. (Hansen's homepage: www.cmap.polytechnique.fr/~nikolaus.hansen/)

References
https://arxiv.org/abs/1604.00772
(Eds.). Handbook of Computational Intelligence, Springer-Verlag, 2015.

See Also
cmaes::cmaes, parma::cmaes

Examples
## Not run:
## Polynomial minimax approximation of data points
## (see the Remez algorithm)
n <- 10; m <- 101 # polynomial of degree 10; no. of data points
xi <- seq(-1, 1, length = m)
yi <- 1 / (1 + (5*xi)^2) # Runge's function
pval <- function(p, x) # Horner scheme
    outer(x, (length(p) - 1):0, "^") %*% p

pfit <- function(x, y, n) # polynomial fitting of degree n
    qr.solve(outer(x, seq(n, 0), "^"), y)

fn1 <- function(p) # objective function
    max(abs(pval(p, xi) - yi))

pf <- pfit(xi, yi, 10) # start with a least-squares fitting
sol1 <- pureCMAES(pf, fn1, rep(-200, 11), rep(200, 11))
zapsmall(sol1$xmin)
# [1] -50.24826 0.00000 135.85352 0.00000 -134.20107 0.00000
# [7] 59.19315 0.00000 -11.55888 0.00000 0.93453

print(sol1$fmin, digits = 10)
# [1] 0.06546780411

## Polynomial fitting in the L1 norm
## (or use LP or IRLS approaches)
fn2 <- function(p)
    sum(abs(pval(p, xi) - yi))

sol2 <- pureCMAES(pf, fn2, rep(-100, 11), rep(100, 11))
zapsmall(sol2$xmin)
# [1] -21.93238 0.00000 62.91083 0.00000 -67.84847 0.00000
# [7] 34.14398 0.00000 -8.11899 0.00000 0.84533

print(sol2$fmin, digits = 10)
# [1] 3.061810639

## End(Not run)

---

**fminviz, flineviz**  **Visualize Function Minimum**

**Description**

Visualizes multivariate functions around a point or along a line between two points in $\mathbb{R}^n$.

**Usage**

```r
fminviz(fn, x0, nlines = 2*length(x0), npoints = 51, scaled = 1.0)
flineviz(fn, x1, x2, npoints = 51, scaled = 0.1)
```
Arguments

- \( fn \) : multivariate function to be visualized.
- \( x_0, x_1, x_2 \) : points in n-dimensional space.
- \( nlines \) : number of lines to plot.
- \( npoints \) : number of points used to plot a line.
- \( scaled \) : scale factor to extend the line(s).

Details

\( \text{fminviz} \) visualizes the behavior of a multivariate function \( fn \) around a point \( x_0 \). It randomly selects \( nlines \) lines through \( x_0 \) in \( \mathbb{R}^n \) and draws the curves of the function along these lines in one graph. Curves that have at least one point below \( fn(x_0) \) are drawn in red, all others in blue. The scale on the x-axis is the Euclidean distance in \( \mathbb{R}^n \). The scale factor can change it.

\( \text{flineviz} \) visualizes the behavior of a multivariate function \( fn \) along the straight line between the points \( x_1 \) and \( x_2 \). Points \( x_1 \) and \( x_2 \) are also plotted.

Value

Plots a line graph and returns NULL (invisibly).

Examples

```r
## Not run:
f1 <- function(x) x[1]^2 - x[2]^2
fminviz(f1, c(0, 0), nlines = 10)

f2 <- function(x) (1 - x[1])^2 + 100*(x[2] - x[1]^2)^2
flineviz(f2, c(0, 0), c(1, 1))
## End(Not run)
```

---

\( \text{hamiltonian} \) : Finds a Hamiltonian path or cycle

Description

A Hamiltonian path or cycle (a.k.a. Hamiltonian circuit) is a path through a graph that visits each vertex exactly once, resp. a closed path through the graph.

Usage

```r
hamiltonian(edges, start = 1, cycle = TRUE)
```
**Arguments**

- **edges**: an edge list describing an undirected graph.
- **start**: vertex number to start the path or cycle.
- **cycle**: Boolean, should a path or a full cycle be found.

**Details**

`hamiltonian()` applies a backtracking algorithm that is relatively efficient for graphs of up to 30–40 vertices. The edge list is first transformed to a list where the i-th component contains the list of all vertices connected to vertex i.

The edge list must be of the form `c(v1, v2, v3, v2, ...)` meaning that there are edges `v1 --> v2, v3 --> v4`, etc., connecting these vertices. Therefore, an edge list has an even number of entries.

If the function returns `NULL`, there is no Hamiltonian path or cycle. The function does not check if the graph is connected or not. And if `cycle = TRUE` is used, then there also exists an edge from the last to the first entry in the resulting path.

If a Hamiltonian cycle exists in the graph it will be found whatever the starting vertex was. For a Hamiltonian path this is different and a successful search may very well depend on the start.

**Value**

Returns a vector containing vertex number of a valid path or cycle, or `NULL` if no path or cycle has been found (i.e., does not exist); If a cycle was requested, there exists an edge from the last to the first vertex in this list of edges.

**Note**

See the igraph package for more information about handling graphs and defining them through edge lists or other constructs.

**Author(s)**

Hans W. Borchers

**References**


**See Also**

Package igraph

**Examples**

```r
## Dodekaeder graph
D20_edges <- c(
  1, 2, 1, 5, 1, 6, 2, 3, 2, 8, 3, 4, 3, 10, 4, 5, 4, 12,
  5, 14, 6, 7, 6, 15, 7, 8, 7, 16, 8, 9, 9, 10, 9, 17, 10, 11,
  11, 12, 11, 17, 10, 9, 9, 10, 11, 12, 11, 8, 7, 6, 15, 7, 8,
  7, 8, 7, 16, 8, 9, 9, 10, 9, 17, 10, 11, 11, 12, 11, 8, 7,
  6, 15, 7, 8, 7, 16, 8, 9, 9, 10, 9, 17, 10, 11, 11, 12, 11)```

```r
D20_path <- hamiltonian(edges = D20_edges, cycle = TRUE)
D20_path
#> [1] 1 2 1 5 1 6 2 3 2 8 3 4 3 10 4 5 4 12 5 14 6
```
hookejeeves

Hooke-Jeeves Minimization Method

Description

An implementation of the Hooke-Jeeves algorithm for derivative-free optimization.
hookejeeves

Usage

hookejeeves(x0, f, lb = NULL, ub = NULL,
  tol = 1e-08,
  target = Inf, maxfeval = Inf, info = FALSE, ...)

Arguments

x0 starting vector.
f nonlinear function to be minimized.
lb, ub lower and upper bounds.
tol relative tolerance, to be used as stopping rule.
target iteration stops when this value is reached.
maxfeval maximum number of allowed function evaluations.
info logical, whether to print information during the main loop.
... additional arguments to be passed to the function.

Details

This method computes a new point using the values of f at suitable points along the orthogonal coordinate directions around the last point.

Value

List with following components:

xmin minimum solution found so far.
fmin value of f at minimum.
fcalls number of function evaluations.
niter number of iterations performed.

Note

Hooke-Jeeves is notorious for its number of function calls. Memoization is often suggested as a remedy.

For a similar implementation of Hooke-Jeeves see the 'dfoptim' package.

References

C.T. Kelley (1999), Iterative Methods for Optimization, SIAM.

See Also

neldermead
## Rosenbrock function

```r
rosenbrock <- function(x) {
  n <- length(x)
  x1 <- x[2:n]
  x2 <- x[1:(n-1)]
  sum(100*(x1-x2^2)^2 + (1-x2)^2)
}
```

```r
hookejeeves(c(0,0,0,0), rosenbrock)
# $xmin
# [1] 1.000000 1.000001 1.000002 1.000004
# $fmin
# [1] 4.774847e-12
# $fcalls
# [1] 2499
# $niter
# [1] 26

hookejeeves(rep(0,4), lb=rep(-1,4), ub=0.5, rosenbrock)
# $xmin
# [1] 0.50000000 0.26221320 0.07797602 0.00608027
# $fmin
# [1] 1.667875
# $fcalls
# [1] 571
# $niter
# [1] 26
```

---

### knapsack

#### 0-1 Knapsack Problem

**Description**

Solves the 0-1 (binary) single knapsack problem.

**Usage**

```r
knapsack(w, p, cap)
```

**Arguments**

- `w`: integer vector of weights.
- `p`: integer vector of profits.
- `cap`: maximal capacity of the knapsack, integer too.
knapsack

Details

knapsack solves the 0-1, or: binary, single knapsack problem by using the dynamic programming approach. The problem can be formulated as:
Maximize \( \sum(x*p) \) such that \( \sum(x*w) \leq cap \), where \( x \) is a vector with \( x[i] = 0 \) or \( 1 \).
Knapsack procedures can even solve subset sum problems, see the examples 3 and 3’ below.

Value

A list with components capacity, profit, and indices.

Author(s)

HwB email: <hwborchers@googlemail.com>

References


See Also

knapsack::knapsack

Examples

# Example 1
p <- c(15, 100, 90, 60, 40, 15, 10, 1)
w <- c(2, 20, 20, 30, 40, 30, 60, 10)
cap <- 102
isis <- knapsack(w, p, cap)
# [1] 1 2 3 4 6 , capacity 102 and total profit 280

## Example 2
p <- c(70, 20, 39, 37, 7, 5, 10)
w <- c(31, 10, 20, 19, 4, 3, 6)
cap <- 50
isis <- knapsack(w, p, cap)
# [1] 1 4 , capacity 50 and total profit 107

## Not run:
## Example 3: subset sum
p <- seq(2, 44, by = 2)*2
w <- p
isis <- knapsack(w, p, 2012)
p[isis$indices] # 16, 36, 64, 144, 196, 256, 324, 400, 576

## Example 3: maximize number of items
# w <- seq(2, 44, by = 2)*2
## Example 4 from Rosetta Code:
```
w = c( 9, 13, 153, 50, 15, 68, 27, 39, 23, 52, 11,
     32, 24, 48, 73, 42, 43, 22, 7, 18, 4, 30)
p = c(150, 35, 200, 160, 60, 45, 60, 40, 30, 10, 70,
     30, 15, 10, 40, 70, 75, 80, 20, 12, 50, 10)
cap = 400
system.time(is <- knapsack(w, p, cap)) # 0.001 sec
```

## End(Not run)

### maxempty

**Maximally Empty Rectangle Problem**

**Description**

Find the largest/maximal empty rectangle, i.e. with largest area, not containing given points.

**Usage**

```
maxempty(x, y, ax = c(0, 1), ay = c(0, 1))
```

**Arguments**

- `x, y` coordinates of points to be avoided.
- `ax, ay` left and right resp. lower and upper constraints.

**Details**

Find the largest or maximal empty two-dimensional rectangle in a rectangular area. The edges of this rectangle have to be parallel to the edges of the enclosing rectangle (and parallel to the coordinate axes). ‘Empty’ means that none of the points given are contained in the interior of the found rectangle.

**Value**

List with `area` and `rect` the rectangle as a vector usable for the `rect` graphics function.

**Note**

The algorithm has a run-time of $O(n^2)$ while there are run-times of $O(n \log(n))$ reported in the literature, utilizing a more complex data structure. I don’t know of any comparable algorithms for the largest empty circle problem.

**Author(s)**

HwB email: <hwborchers@googlemail.com>
**maxquad**

The MAXQUAD Test Function

**Description**

Lemarechal’s MAXQUAD optimization test function.

**Usage**

```r
maxquad(n, m)
```

**Arguments**

- `n`: number of variables of the generated test function.
- `m`: number of functions to compete for the maximum.

**Details**

MAXQUAD actually is a family of minimax functions, parametrized by the number `n` of variables and the number `m` of functions whose maximum it is.

**References**


**See Also**

`Hmisc::largest.empty` with a Fortran implementation of this code.

**Examples**

```r
N <- 100; set.seed(8237)
x <- runif(N); y <- runif(N)
R <- maxempty(x, y, c(0,1), c(0,1))
R
# $area
# [1] 0.08238793
# $rect
# [1] 0.7023670 0.1797339 0.8175771 0.8948442

## Not run:
plot(x, y, pch="+", xlim=c(0,1), ylim=c(0,1), col="darkgray",
     main = "Maximally empty rectangle")
rect(0, 0, 1, 1, border = "red", lwd = 1, lty = "dashed")
do.call(rect, as.list(R$rect))
grid()
## End(Not run)
```
Value

Returns a list with components fn the generated test function of n variables, and gr the corresponding (analytical) gradient function.

References


Examples

# Test function of 5 variables, defined as maximum of 5 smooth functions
maxq <- maxquad(5, 5)
fnMaxquad <- maxq$fn
grMaxquad <- maxq$gr
# shor

maxsub Maximal Sum Subarray

Description

Find a subarray with maximal positive sum.

Usage

maxsub(x, inds = TRUE)

maxsub2d(A)

Arguments

x numeric vector.
A numeric matrix
inds logical; shall the indices be returned?

Details

maxsub finds a contiguous subarray whose sum is maximally positive. This is sometimes called Kadane’s algorithm. maxsub will use a very fast version with a running time of \(O(n)\) where \(n\) is the length of the input vector \(x\).

maxsub2d finds a (contiguous) submatrix whose sum of elements is maximally positive. The approach taken here is to apply the one-dimensional routine to summed arrays between all rows of \(A\). This has a run-time of \(O(n^3)\), though a run-time of \(O(n^2 \log n)\) seems possible see the reference below. maxsub2d can solve a 100-by-100 matrix in a few seconds – but beware of bigger ones.
**Value**

Either just a maximal sum, or a list this sum as component sum plus the start and end indices as a vector `inds`.

**Note**

In special cases, the matrix `A` may be sparse or (as in the example section) only have one nonzero element in each row and column. Expectation is that there may exists a more efficient (say `O(n^2)`) algorithm in these special cases.

**Author(s)**

HwB <hwborchers@googlemail.com>

**References**


**Examples**

```r
## Find a maximal sum subvector
set.seed(8237)
x <- rnorm(1e6)
system.time(res <- maxsub(x, inds = TRUE))
res
```

```r
## Standard example: Find a maximal sum submatrix
A <- matrix(c(0,-2,-7,0, 9,2,-6,2, -4,1,-4,1, -1,8,0,2),
nrow = 4, ncol = 4, byrow = TRUE)
maxsub2d(A)
# $sum: 15
# $inds: 2 4 1 2 , i.e., rows = 2..4, columns = 1..2
```

```r
## Not run:
## Application to points in the unit square:
set.seed(723)
N <- 50; w <- rnorm(N)
x <- runif(N); y <- runif(N)
col <- ifelse (w >= 0, "blue", "red")
plot(x, y, pch = 20, col = clr, xlim = c(0, 1), ylim = c(0, 1))
x <- unique(sort(x)); ns <- length(xs)
X <- c(0, ((xs[1:(ns-1)] + xs[2:ns])/2), 1)
y <- unique(sort(y)); ms <- length(ys)
Y <- c(0, ((ys[1:(ns-1)] + ys[2:ns])/2), 1)
abline(v = X, col = "gray")
abline(h = Y, col = "gray")
A <- matrix(0, N, N)
```
mknapsack

```r
xi <- findInterval(x, X); yi <- findInterval(y, Y)
for (i in 1:N) A[y[i], xi[i]] <- w[i]

msr <- maxsub2d(A)

## End(Not run)
```

---

### Description

Solves the 0-1 (binary) multiple knapsack problem.

### Usage

```r
mknapsack(w, p, cap)
```

### Arguments

- **w**: vector of (positive) weights.
- **p**: vector of (positive) profits.
- **cap**: vector of capacities of different knapsacks.

### Details

Solves the 0-1 multiple knapsack problem for a set of profits and weights. A multiple 0-1 knapsack problem can be formulated as:

\[
\text{maximize } v^{\star} = p(1) \times (x(1,1) + \ldots + x(m,1)) + \ldots \ldots + p(n) \times (x(1,n) + \ldots + x(m,n)) \text{ subject to } w(1) \times x(i,1) + \ldots + w(n) \times x(i,n) \leq \text{cap}(i) \text{ for } i=1,\ldots,m \times x(1,j) + \ldots + x(m,j) \leq 1 \text{ for } j=1,\ldots,n \times (i,j) \leq 0 \text{ or } 1 \text{ for } i=1,\ldots,m, j=1,\ldots,n.
\]

The multiple knapsack problem is reformulated as a linear program and solved with the help of package lpSolve.

This function can be used for the single knapsack problem as well, but the 'dynamic programming’ version in the knapsack function is faster (but: allows only integer values).

The solution found is most often not unique and may not be the most compact one. In the future, we will attempt to 'compactify’ through backtracking. The number of backtracks will be returned in list element bs.

### Value

A list with components, ksack the knapsack numbers the items are assigned to, value the total value/profit of the solution found, and bs the number of backtracks used.
mknapsack

Note

Contrary to earlier versions, the sequence of profits and weights has been interchanged: first the weights, then profits.

The compiled version was transferred to the knapsack package on R-Forge (see project ‘optimist’).

References


See Also

Other packages implementing knapsack routines.

Examples

## Example 1: single knapsack
w <- c(2, 20, 20, 30, 40, 30, 60, 10)
p <- c(15, 100, 90, 60, 40, 15, 10, 1)
cap <- 102
(is <- mknapsack(w, p, cap))
which(is$ksack == 1)
# [1] 1 2 3 4 6 , capacity 102 and total profit 280

## Example 2: multiple knapsack
w <- c(40, 60, 30, 40, 20, 5)
p <- c(110, 150, 70, 80, 30, 5)
cap <- c(85, 65)
is <- mknapsack(w, p, cap)
# kps 1: 1,4; kps 2: 2,6; value: 345

## Example 3: multiple knapsack
p <- c(78, 35, 89, 36, 75, 74, 79, 80, 16)
w <- c(18, 9, 23, 20, 59, 61, 70, 75, 76, 30)
cap <- c(103, 156)
is <- mknapsack(w, p, cap)
# kps 1: 3,4,5; kps 2: 1,6,9; value: 452

## Not run:
# How to Cut Your Planks with R
# R-bloggers, Rasmus Baath, 2016-06-12
#
# This is application of multiple knapsacks to cutting planks into pieces.
planks_we_have <- c(120, 137, 220, 420, 480)
s <- mknapsack(planks_we.want, planks_we.want + 1, planks_we.have)
s$ksack
## [1] 5 5 5 5 3 5 5 4 1 5 4 5 3 2 4

# Solution w/o backtracking
# bin 1 : 103 | Rest: 17
# bin 2 : 135 | Rest: 2
# bin 3 : 79 + 135 | Rest: 6
# bin 4 : 103 + 135 + 160 | Rest: 22
# bin 5 : 4*19 + 2*79 + 103 + 135 | Rest: 8
#
# Solution with reversing the bins (bigger ones first)
# bin 1 : 103 | Rest: 4
# bin 2 : 2*19 + 79 | Rest: 20
# bin 3 : 79 + 135 | Rest: 6
# bin 4 : 2*19 + 79 + 135 + 160 | Rest: 8
# bin 5 : 2*103 + 2*135 | Rest: 17
#
# Solution with backtracking (compactification)
# sol = c(1, 4, 4, 1, 1, 3, 4, 5, 5, 5, 5, 4, 2, 3, 4)
# bin 1 : 2*19 + 79 | Rest: 3
# bin 2 : 135 | Rest: 2
# bin 3 : 79 + 135 | Rest: 6
# bin 4 : 2*19 + 79 + 135 + 160 | Rest: 8
# bin 5 : 3*103 + 135 | Rest: 36

## End(Not run)

---

**neldermead**

*Nelder-Mead Minimization Method*

**Description**

An implementation of the Nelder-Mead algorithm for derivative-free optimization / function minimization.

**Usage**

```r
neldermead( fn, x0, ..., adapt = TRUE,
            tol = 1e-10, maxfeval = 10000,
            step = rep(1.0, length(x0)))

neldermeadb(fn, x0, ..., lower, upper, adapt = TRUE,
            tol = 1e-10, maxfeval = 10000,
            step = rep(1, length(x0)))
```

**Arguments**

- `fn`: nonlinear function to be minimized.
- `x0`: starting point for the iteration.
- `adapt`: logical; adapt to parameter dimension.
tol     terminating limit for the variance of function values; can be made *very* small, like tol=1e-50.
maxfeval maximum number of function evaluations.
step     size and shape of initial simplex; relative magnitudes of its elements should reflect the units of the variables.
...     additional arguments to be passed to the function.
lower, upper lower and upper bounds.

Details
Also called a ‘simplex’ method for finding the local minimum of a function of several variables. The method is a pattern search that compares function values at the vertices of the simplex. The process generates a sequence of simplices with ever reducing sizes.

The simplex function minimisation procedure due to Nelder and Mead (1965), as implemented by O’Neill (1971), with subsequent comments by Chambers and Ertel 1974, Benyon 1976, and Hill 1978. For another elaborate implementation of Nelder-Mead in R based on Matlab code by Kelley see package ‘dfoptim’.

eeldermead can be used up to 20 dimensions (then ‘tol’ and ‘maxfeval’ need to be increased). With adapt=TRUE it applies adaptive coefficients for the simplicial search, depending on the problem dimension – see Fuchang and Lixing (2012). This approach especially reduces the number of function calls.

With upper and/or lower bounds, neldermeadb applies transfinite to define the function on all of R^n and to retransform the solution to the bounded domain. Of course, if the optimum is near to the boundary, results will not be as accurate as when the minimum is in the interior.

Value
List with following components:
xmin minimum solution found.
fmin value of f at minimum.
fcount number of iterations performed.
restarts number of restarts.
errmess error message

Note
Original FORTRAN77 version by R O’Neill; MATLAB version by John Burkardt under LGPL license. Re-implemented in R by Hans W. Borchers.

References
See Also

hookejeeves

Examples

## Classical tests as in the article by Nelder and Mead

# Rosenbrock's parabolic valley
rpv <- function(x) 100*(x[2] - x[1]^2)^2 + (1 - x[1])^2
x0 <- c(-2, 1)
neldermead(rpv, x0)  # 1 1

# Fletcher and Powell's helic valley
fphv <- function(x)
  100*(x[3] - 10*atan2(x[2], x[1])/(2*pi))^2 +
x0 <- c(-1, 0, 0)
neldermead(fphv, x0)  # 1 0 0

# Powell's Singular Function (PSF)
psf <- function(x) (x[1] + 10*x[2])^2 + 5*(x[3] - x[4])^2 +
x0 <- c(3, -1, 0, 1)
neldermead(psf, x0)  # 0 0 0 0, needs maximum number of function calls

# Bounded version of Nelder-Mead
lower <- c(-Inf, 0, 0)
upper <- c(Inf, 0.5, 1)
x0 <- c(0, 0.1, 0.1)
neldermeadb(fnRosenbrock, c(0, 0.1, 0.1), lower = lower, upper = upper)
# $xmin = c(0.7085595, 0.5000000, 0.2500000)
# $fmin = 0.3353605
# $fcount = 1426085
# elapsed time is 96.008000 seconds

## Not run:
# Can run Rosenbrock's function in 30 dimensions in one and a half minutes:
neldermead(fnRosenbrock, rep(0, 30), tol=1e-20, maxfeval=10^7)
# $xmin
# [1] 0.9999998 1.0000004 1.0000000 1.0000000 1.0000000 1.0000000
# [7] 1.0000000 0.9999997 0.9999997 0.9999997 0.9999997 1.0000000
# [13] 0.9999999 0.9999999 0.9999999 0.9999999 0.9999999 0.9999999
# [19] 0.9999999 1.0000000 0.9999998 1.0000000 0.9999993 0.9999999
# [25] 1.0000000 0.9999996 0.9999995 0.9999999 0.9999973 0.9999947
# $fmin
# [1] 5.617352e-10
# $fcount
# [1] 1426085
# elapsed time is 96.008000 seconds
occurs

## End(Not run)

---

occurs  Finding Subsequences

### Description

Find subsequences of (integer) sequences.

### Usage

`occurs(subseq, series)`

### Arguments

- `subseq`: vector of integers.
- `series`: vector of integers.

### Details

If `m` and `n` are the lengths of `s` and `S` resp., `occurs(s, S)` determines all positions `i` such that `s == S[i, ..., i+m-1]`.

The code is vectorized and relatively fast. It is intended to complement this with an implementation of Rabin-Karp, and possibly Knuth-Morris-Pratt and Boyer-Moore algorithms.

### Value

Returns a vector of indices.

### Examples

```r
## Examples
patrn <- c(1,2,3,4)
exmpl <- c(3,3,4,2,3,1,2,3,4,8,8,23,1,2,3,4,8,8,23,1,2,3,4,8,8,23,1,2,3,4)
occurs(patrn, exmpl)
## [1] 6 13 23

## Not run:
set.seed(2437)
p = sample(1:20, 1000000, replace=TRUE)
system.time(i <- occurs(c(1,2,3,4,5), p)) #=> [1] 799536
## user  system elapsed
## 0.017 0.000  0.017 [sec]

## End(Not run)
```
setcover

Set cover problem

Description
Solves the Set Cover problem as an integer linear program.

Usage
setcover(Sets, weights)

Arguments
Sets matrix of 0s and 1s, each line defining a subset.
weights numerical weights for each subset.

Details
The Set Cover problems attempts to find in subsets (of a 'universe') a minimal set of subsets that
still covers the whole set.
Each line of the matrix Sets defines a characteristic function of a subset. It is required that each
element of the universe is contained in at least one of these subsets.
The problem is treated as an Integer Linear Program (ILP) and solved with the lp solver in lpSolve.

Value
Returns a list with components sets, giving the indices of subsets, and objective, the sum of
weights of subsets present in the solution.

References
See the Wikipedia article on the "set cover problem".

See Also
knapsack

Examples
# Define 12 subsets of universe {1, ..., 10}.
set.seed(7*11*13)
A <- matrix(sample(c(0,1), prob = c(0.8,0.2), size = 120, replace =TRUE),
nrow = 12, ncol = 10)
sol <- setcover(Sets = A, weights = rep(1, 12))
sol
## $sets
## [1]  1  2  9 12
## $no.sets
Description

Test functions for global optimization posed for the SIAM 100-digit challenge in 2002 by Nick Trefethen, Oxford University, UK.

Usage

\texttt{fnTrefethen(p2)}
\texttt{fnWagon(p3)}

Arguments

\begin{itemize}
  \item \texttt{p2} Numerical vector of length 2.
  \item \texttt{p3} Numerical vector of length 3.
\end{itemize}

Details

These are highly nonlinear and oscillating functions in two and three dimensions with thousands of local mimima inside the unit square resp. cube (i.e., [-1, 1] x [-1, 1] or [-1, 1] x [-1, 1] x [-1, 1]).

Value

Function value is a single real number.

Author(s)

HwB hwborchers@gmail.com

References

Examples

```r
x <- 2*runif(5) - 1
fnTrefethen(x)
fnWagon(x)
```

```r
## Not run:
T <- matrix(NA, nrow=1001, ncol=1001)
for (i in 1:1001) {
  for (j in 1:1001) {
    T[i, j] <- fnTrefethen(c(x[i], y[j]))
  }
}
image(x, y, T)
contour(x, y, T, add=TRUE)
## End(Not run)
```

---

**simpleDE**

*Simple Differential Evolution Algorithm*

**Description**

Simple Differential Evolution for Minimization.

**Usage**

```r
simpleDE(fun, lower, upper, N = 64, nmax = 256, r = 0.4,
         confined = TRUE, log = FALSE)
```

**Arguments**

- `fun` : the objective function to be minimized.
- `lower` : vector of lower bounds for all coordinates.
- `upper` : vector of upper bounds for all coordinates.
- `N` : population size.
- `nmax` : bound on the number of generations.
- `r` : amplification factor.
- `confined` : logical; stay confined within bounds.
- `log` : logical; shall a trace be printed.

**Details**

Evolutionary search to minimize a function: For points in the current generation, children are formed by taking a linear combination of parents, i.e., each member of the next generation has the form

\[ p_1 + r(p_2 - p_3) \]

where the \( p_i \) are members of the current generation and \( r \) is an amplification factor.
Value

List with the following components:

- fmin: function value at the minimum found.
- xmin: numeric vector representing the minimum.
- nfeval: number of function calls.

Note

Original Mathematica version by Dirk Laurie in the SIAM textbook. Translated to R by Hans W Borchers.

Author(s)

HwB <hwborchers@googlemail.com>

References


See Also

simpleEA, DEoptim in the ‘DEoptim’ package.

Examples

```r
simpleDE(fnTrefethen, lower = c(-1,-1), upper = c(1,1))
# $fmin
# [1] -3.306869
# $xmin
# [1] -0.02440308 0.21061243 # this is the true global optimum!
```

Description

Simple Evolutionary Algorithm for Minimization.

Usage

```r
simpleEA(fn, lower, upper, N = 100, ..., con = 0.1, new = 0.05, 
          tol = 1e-10, eps = 1e-07, scl = 1/2, confined = FALSE, log = FALSE)
```
Arguments

- `fn`: the objective function to be minimized.
- `lower`: vector of lower bounds for all coordinates.
- `upper`: vector of upper bounds for all coordinates.
- `N`: number of children per parent.
- `...`: additional parameters to be passed to the function.
- `con`: percentage of individuals concentrating to the best parents.
- `new`: percentage of new individuals not focussed on existing parents.
- `tol`: tolerance; if in the last three loops no better individuals were found up to this tolerance, stop.
- `eps`: grid size bound to be reached.
- `scl`: scaling factor for shrinking the grid.
- `confined`: logical; shall the set of individuals be strictly respect the boundary? Default: FALSE.
- `log`: logical, should best solution found be printed per step.

Details

Evolutionary search to minimize a function: For each point in the current generation, \( n \) random points are introduced and the \( n \) best results of each generation (and its parents) are used to form the next generation.

The scale shrinks the generation of new points as the algorithm proceeds. It is possible for some children to lie outside the given rectangle, and therefore the final result may lie outside the unit rectangle well. (TO DO: Make this an option.)

Value

List with the following components:

- `par`: numeric vector representing the minimum found.
- `val`: function value at the minimum found.
- `fun.calls`: number of function calls made.
- `rel.scl`: last scaling factor indicating grid size in last step.
- `rel.tol`: relative tolerance within the last three minima found.

Note


Author(s)

HwB <hwborchers@googlemail.com>
References


See Also

DEoptim in the ‘DEoptim’ package.

Examples

```r
simpleEA(fnTrefethen, lower=c(-1,-1), upper=c(1,1), log=FALSE)
# $par
#  [1] -0.02440310 0.21061243 # this is the true global optimum!
# $val
#  [1] -3.306869
```

subsetsum

Subset Sum Problem

Description

Subset sum routine for positive integers.

Usage

```r
subsetsum(S, t, method = "greedy")
```

```r
sss_test(S, t)
```

Arguments

- **S**: vector of positive integers.
- **t**: target value, bigger than all items in S.
- **method**: can be “greedy” or “dynamic”, where “dynamic” stands for the dynamic programming approach.

Details

subsetsum is searching for a set of elements in S that sum up to t by continuously adding more elements of S.

It is not required that S is decreasingly sorted. But for reasons of efficiency and smaller execution times it is urgently recommended to sort the item set in decreasing order. See the examples to find out how to handle your data.

The first components will be preferred, i.e., if S is decreasing, the sum with larger elements will be found, if increasing, the sum with smaller elements. Because of timing considerations, the default is to sort decreasingly before processing.
The dynamic method may be faster for large sets, but will also require much more memory if the target value is large.

`sss_test` will find the biggest number below or equal to \( t \) that can be expressed as a sum of items in \( S \). It will not return any indices. It can be quite fast, though it preprocesses the set \( S \) to be sorted decreasingly, too.

**Value**

List with the target value, if reached, and vector of indices of elements in \( S \) that sum up to \( t \).

If no solution is found, the dynamic method will return indices for the largest value below the target, the greedy method will return NULL.

`sss_test` will simply return maximum sum value found.

**Note**

A compiled version – and much faster, in Fortran – can be found in package ’knapsack’ (R-Forge, project ’optimist’) as `subsetsum`. A recursive version, returning *all* solutions, is much too slow in R, but is possible in Julia and can be asked from the author.

**Author(s)**

HwB email: <hwborchers@googlemail.com>

**References**


**See Also**

`maxsub`

**Examples**

```r
# Not run:
t <- 5842
S <- c(267, 493, 869, 961, 1000, 1153, 1246, 1598, 1766, 1922)

# S is not decreasingly sorted, so ...
o <- order(S, decreasing = TRUE)
So <- S[o]  # So is decreasingly sorted

sol <- subsetsum(So, t)  # $inds: 2 4 6 7 8 w.r.t. So
is <- o[sol$inds]  # is: 9 7 5 4 3 w.r.t. S
sum(S[is])  # 5842

amount <- 4748652
products <-
c(38500, 30500, 30500, 30500, 42000, 42000, 42000, 42000, 42000, 42000, 42000, 42000, 42000, 71040, 90900,
    42000, 42000, 42000, 42000, 42000, 42000, 42000, 42000, 71040, 90900,
```
# Testfunctions

Optimization Test Functions

Description

Simple and often used test function defined in higher dimensions and with analytical gradients, especially suited for performance tests. Analytical gradients, where existing, are provided with the gr prefix. The dimension is determined by the length of the input vector.

Usage

fnRosenbrock(x)
gRosenbrock(x)
fnRastrigin(x)
gRastrigin(x)
fnNesterov(x)
gNesterov(x)
fnNesterov1(x)
Arguments

\( x \) numeric vector of a certain length.

Details

**Rosenbrock** – Rosenbrock’s famous valley function from 1960. It can also be regarded as a least-squares problem:

\[
\sum_{i=1}^{n-1} (1 - x_i)^2 + 100(x_{i+1} - x_i^2)^2
\]

No. of Vars.: \( n \geq 2 \)
Bounds: \(-5.12 \leq x_i \leq 5.12\)
Local minima: at \( f(-1, 1, \ldots, 1) \) for \( n \geq 4 \)
Minimum: 0.0
Solution: \( x_i = 1, i = 1:n \)

**Nesterov** – Nesterov’s smooth adaptation of Rosenbrock, based on the idea of Chebyshev polynomials. This function is even more difficult to optimize than Rosenbrock’s:

\[
(x_1 - 1)^2 / 4 + \sum_{i=1}^{n-1} (1 + x_{i+1} - 2x_i^2)
\]

No. of Vars.: \( n \geq 2 \)
Bounds: \(-5.12 \leq x_i \leq 5.12\)
Local minima: ?
Minimum: 0.0
Solution: \( x_i = 1, i = 1:n \)

**Nesterov1** – Similar to Nesterov, except the terms added are taken with absolute value, which makes this function nonsmooth and painful for gradient-based optimization routines; no gradient provided.

**Rastrigin** – Rastrigin’s function is a famous, non-convex example from 1989 for global optimization. It is a typical example of a multimodal function with many local minima:

\[
10n + \sum_{i=1}^{n} (x_i^2 - 10 \cos(2\pi x_i))
\]
transfinite

transfinite

Hald – Hald’s function is a typical example of a non-smooth test function, from Hald and Madsen in 1981.

\[
\max_{1 \leq i \leq n} \frac{x_1 + x_2 t_i}{1 + x_3 t_i + x_4 t_i^2 + x_5 t_i^3} - \exp(t_i)
\]

where \( t_i = -1 + (i - 1)/10 \) for \( 1 \leq i \leq 21 \).

No. of Vars.: \( n = 5 \)
Bounds: \( -1 \leq x_i \leq 1 \)
Local minima: ?
Minimum: 0.0001223713
Solution: \((0.99987763, 0.25358844, -0.74660757, 0.24520150, -0.03749029)\)

Shor – Shor’s function is another typical example of a non-smooth test function, a benchmark for Shor’s R-algorithm.

Value

Returns the values of the test function resp. its gradient at that point. If an analytical gradient is not available, a function computing the gradient numerically will be provided.

References

Search the Internet.

Examples

\[ x <- \text{runif}(5) \]
\[ \text{fnHald}(x); \text{grHald}(x) \]

# Compare analytical and numerical gradient
\[ \text{shor_gr} <- \text{function(x) adagio:::ns.grad(fnShor, x)} \quad \# \text{internal gradient} \]
\[ \text{grShor}(x); \text{shor_gr}(x) \]

transfinite

Boxed Region Transformation

Description

Transformation of a box/bound constrained region to an unconstrained one.
Usage

transfinite(lower, upper, n = length(lower))

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>lower, upper</td>
<td>lower and upper box/bound constraints.</td>
</tr>
<tr>
<td>n</td>
<td>length of upper, lower if both are scalars, to which they get repeated.</td>
</tr>
</tbody>
</table>

Details

Transforms a constraint region in \( \mathbb{R}^n \) space bijectively to the unconstrained \( \mathbb{R}^n \) space, applying a \( \text{atanh} \) resp. \( \text{exp} \) transformation to each single variable that is bound constraint.

It provides two functions, \( h: B = \{ x \in \mathbb{R}^n : \text{lower} \leq x \leq \text{upper} \} \rightarrow \mathbb{R}^n \) and its inverse \( h^{-1} \). These functions can, for example, be used to add box/bound constraints to a constrained optimization problem that is to be solved with a (nonlinear) solver not allowing constraints.

Value

Returns to functions as components \( h \) and \( h^{-1} \) of a list.

Note

Based on an idea of Ravi Varadhan, intrinsically used in his implementation of Nelder-Mead in the ‘dfoptim’ package.

For positivity constraints, \( x \geq 0 \), this approach is considered to be numerically more stable than \( x \rightarrow \exp(x) \) or \( x \rightarrow x^2 \).

Examples

```r
lower <- c(-Inf, 0, 0)
upper <- c( Inf, 0.5, 1)
Tf <- transfinite(lower, upper)

h <- Tf$h; hinv <- Tf$hinv

# Not run:
# Solve Rosenbrock with one variable restricted
rosen <- function(x) {
  n <- length(x)
  x1 <- x[2:n]; x2 <- x[1:(n-1)]
  sum(100*(x1-x2^2)^2 + (1-x2)^2)
}

f <- function(x) rosen(hinv(x)) # f must be defined on all of \( \mathbb{R}^n \)
x0 <- c(0.1, 0.1, 0.1) # starting point not on the boundary!
nm <- nelder_mead(h(x0), f) # unconstraint Nelder-Mead
hinv(nm$xmin); nm$fmin # box/bound constraint solution

# [1] 0.7085596 0.5000000 0.2500004
# [1] 0.3353605

# End(Not run)
```
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